10540245

result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:37:14 ON 27 APR 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:37:20 ON 27 APR 2007
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STRUCTURE FILE UPDATES: 26 APR 2007 HIGHEST RN 933069-51-3
DICTIONARY FILE UPDATES: 26 APR 2007 HIGHEST RN 933069-51-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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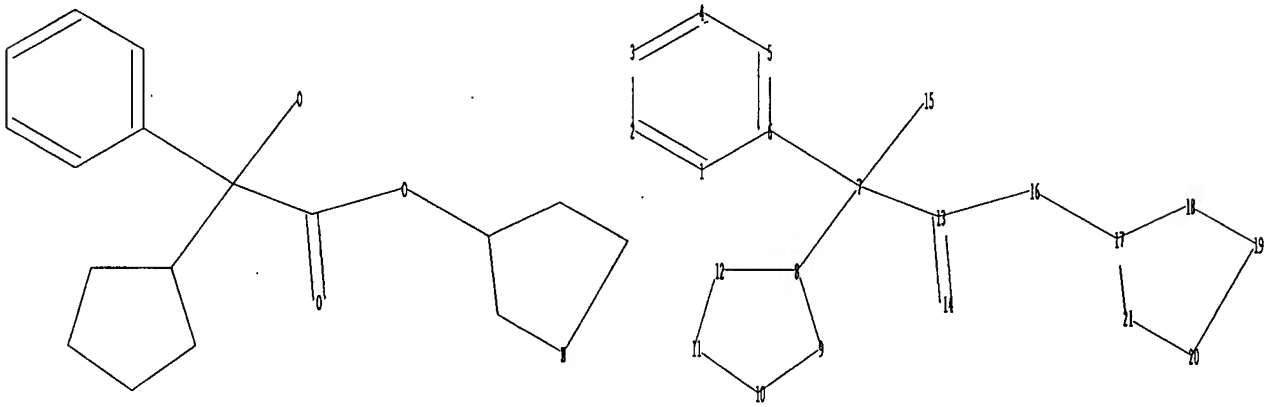
http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10540245f.str



chain nodes :
7 13 14 15 16
ring nodes :

Karen Cheng

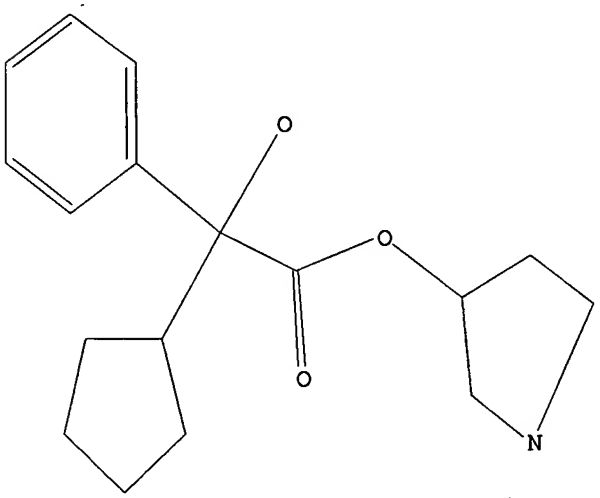
10540245

1 2 3 4 5 6 8 9 10 11 12 17 18 19 20 21
chain bonds :
6-7 7-8 7-13 7-15 13-14 13-16 16-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19
19-20 20-21
exact/norm bonds :
7-15 13-14 13-16 16-17 19-20 20-21
exact bonds :
6-7 7-8 7-13 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 8 : 17 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 14:37:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 293 TO ITERATE

100.0% PROCESSED 293 ITERATIONS 187 ANSWERS
SEARCH TIME: 00.00.01

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10540245

L2 187 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY 172.10 TOTAL SESSION 172.31
FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 14:37:40 ON 27 APR 2007
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FILE COVERS 1907 - 27 Apr 2007 VOL 146 ISS 19
FILE LAST UPDATED: 26 Apr 2007 (20070426/ED)

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http://www.cas.org/infopolicy.html

=> s l2
L3 345 L2

=> fil stng
COST IN U.S. DOLLARS SINCE FILE ENTRY 0.47 TOTAL SESSION 172.78
FULL ESTIMATED COST

FILE 'STNGUIDE' ENTERED AT 14:38:30 ON 27 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Apr 20, 2007 (20070420/UP).

=> fil reg
COST IN U.S. DOLLARS SINCE FILE ENTRY 0.12 TOTAL SESSION 172.90
FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:39:51 ON 27 APR 2007
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STRUCTURE FILE UPDATES: 26 APR 2007 HIGHEST RN 933069-51-3
DICTIONARY FILE UPDATES: 26 APR 2007 HIGHEST RN 933069-51-3

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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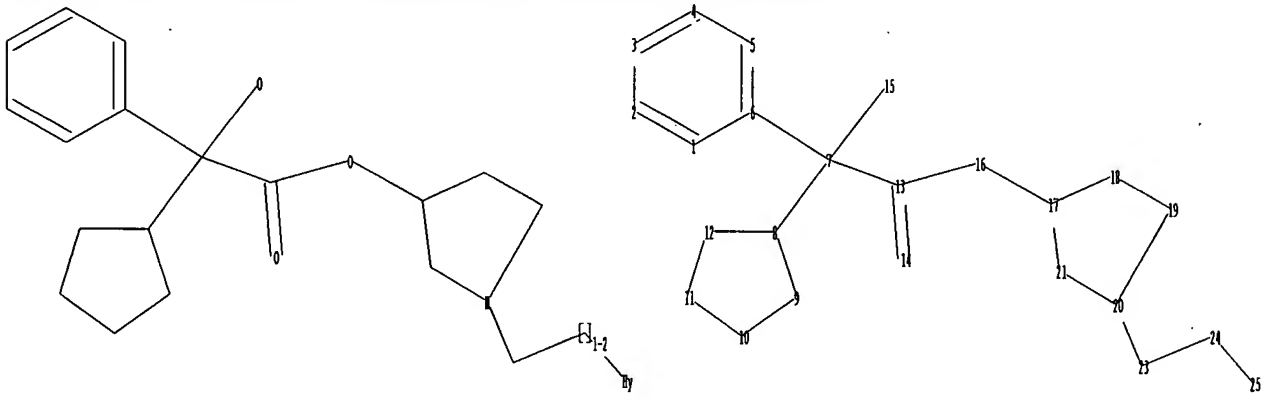
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10540245g.str



chain nodes :
7 13 14 15 16 23 24 25
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 17 18 19 20 21
chain bonds :
6-7 7-8 7-13 7-15 13-14 13-16 16-17 20-23 23-24 24-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19 19-20 20-21
exact/norm bonds :
7-15 13-14 13-16 16-17 19-20 20-21 20-23 24-25
exact bonds :
6-7 7-8 7-13 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19 23-24
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 8 : 17 :

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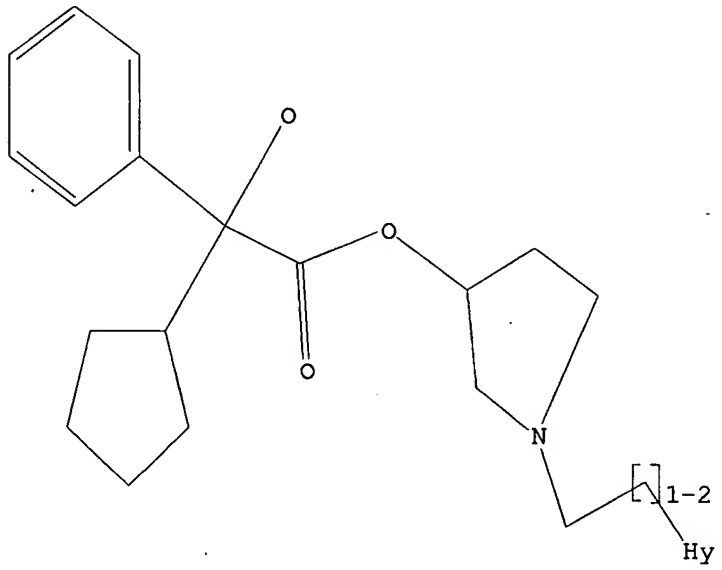
10540245

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 23:CLASS 24:CLASS 25:Atom

L4 STRUCTURE UPLOADED

=> d
L4 HAS NO ANSWERS
L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> d his

(FILE 'HOME' ENTERED AT 14:37:14 ON 27 APR 2007)

FILE 'REGISTRY' ENTERED AT 14:37:20 ON 27 APR 2007
L1 STRUCTURE UPLOADED
L2 187 S L1 FULL

FILE 'CAPLUS' ENTERED AT 14:37:40 ON 27 APR 2007
L3 345 S L2

FILE 'STNGUIDE' ENTERED AT 14:38:30 ON 27 APR 2007

FILE 'REGISTRY' ENTERED AT 14:39:51 ON 27 APR 2007
L4 STRUCTURE UPLOADED

=> s l4 full sub=l2

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10540245

FULL SUBSET SEARCH INITIATED 14:40:20 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 171 TO ITERATE

100.0% PROCESSED 171 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

L5 4 SEA SUB=L2 SSS FUL L4

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	41.10	214.00

FILE 'CAPLUS' ENTERED AT 14:40:25 ON 27 APR 2007
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FILE COVERS 1907 - 27 Apr 2007 VOL 146 ISS 19
FILE LAST UPDATED: 26 Apr 2007 (20070426/ED)

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=> s l5
L6 1 L5

=> d ibib abs hitstr tot

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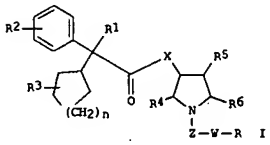
L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:546475 CAPLUS
DOCUMENT NUMBER: 141:106362
TITLE: Preparation of 1-substituted-3-pyrrolidine derivatives as muscarinic receptor antagonists
INVENTOR(S): Mehta, Anita; Gupta, Jang Bahadur; Sarma, Pakala Kumara Savithru
PATENT ASSIGNEE(S): Ranbaxy Laboratories Limited, India
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

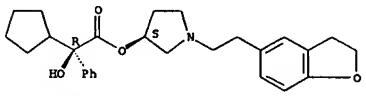
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056767	A1	20040708	WO 2002-IB5590	20021223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002347552	A1	20040714	AU 2002-347552	20021223
EP 1583741	A1	20051012	EP 2002-783480	20021223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2006194862	A1	20060831	US 2006-540245	20060207
PRIORITY APPLN. INFO.:			WO 2002-IB5590 A	20021223

OTHER SOURCE(S): CASREACT 141:106362; MARPAT 141:106362
GI



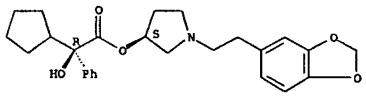
AB Title muscarinic receptor antagonists I (X = O, NH, etc.; R1 = OH, etc.; R2 = H, halo, alkyl; R3 = H, OH, etc.; R4, R5, R6 = H, alkyl; ; Z = CH2, SO2, carbonyl; W = alkylene, etc.; R = alkyl, aryl, etc.), useful for the

L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 719278-75-8 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[2-(1,3-benzodioxol-5-yl)ethyl]-3-pyrrolidinyl ester, (αR)- (9CI) (CA INDEX NAME)

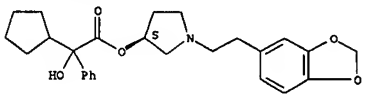
Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

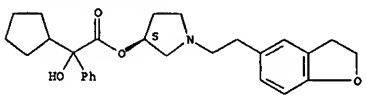
L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
treatment of various diseases of the respiratory, urinary and gastrointestinal systems mediated through muscarinic receptors, are prepd. The affinity of these compds. for M2 and M3 muscarinic receptor subtype was tested. For example, (3S)-1-benzylpyrrolidin-3-yl cyclopentyl(hydroxy)phenylacetate was prepd. and had pKi = 6.13/7.17 for the M2 and M3 receptor subtype resp.
IT 719278-62-3P 719278-63-4P 719278-74-7P
719278-75-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-substituted-3-pyrrolidine derivs. as muscarinic receptor
antagonists)
RN 719278-62-3 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[2-(1,3-benzodioxol-5-yl)ethyl]-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 719278-63-4 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[2-(2,3-dihydro-5-benzofuranyl)ethyl]-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

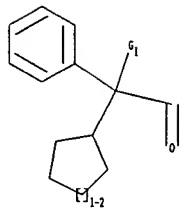
Absolute stereochemistry.

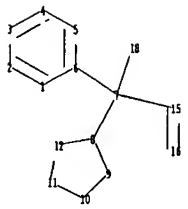


RN 719278-74-7 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[2-(2,3-dihydro-5-benzofuranyl)ethyl]-3-pyrrolidinyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10540245





chain nodes :
7 15 16 18
ring nodes :
1 2 3 4 5 6 8 9 10 11 12
chain bonds :
6-7 7-8 7-15 7-18 15-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12
exact/norm bonds :
7-18 15-16
exact bonds :
6-7 7-8 7-15 8-9 8-12 9-10 10-11 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 8 :

G1:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 15:CLASS 16:CLASS 18:CLASS

L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS

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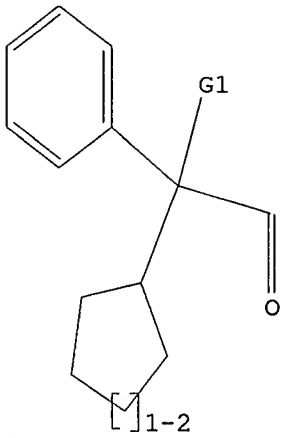
10540245

L3 STR



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=> s l3
SAMPLE SEARCH INITIATED 14:46:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 202 TO ITERATE

100.0% PROCESSED 202 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.04

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3188 TO 4892
PROJECTED ANSWERS: 2231 TO 3689

L4 50 SEA SSS SAM L3

=> s l3 full
FULL SEARCH INITIATED 14:47:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4093 TO ITERATE

100.0% PROCESSED 4093 ITERATIONS 3003 ANSWERS
SEARCH TIME: 00.00.01

L5 3003 SEA SSS FUL L3

=> fil stng

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	344.65	344.86

FILE 'STNGUIDE' ENTERED AT 14:47:06 ON 13 MAR 2007

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10540245

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 9, 2007 (20070309/UP).

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	345.28

FILE 'REGISTRY' ENTERED AT 14:51:18 ON 13 MAR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 MAR 2007 HIGHEST RN 926069-79-6
DICTIONARY FILE UPDATES: 12 MAR 2007 HIGHEST RN 926069-79-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10540245b.str

chain nodes :
7 15 16 18 20 21 22 23 26 27 28
ring nodes :

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10540245

1 2 3 4 5 6 8 9 10 11 12 34 35 36 37 38
chain bonds :
6-7 7-8 7-15 7-18 15-16 15-20 20-34 21-22 22-23 26-27 27-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 34-35 34-38 35-36
36-37 37-38
exact/norm bonds :
7-18 15-16 15-20 20-34 22-23 26-27 34-35 34-38 35-36 36-37 37-38
exact bonds :
6-7 7-8 7-15 8-9 8-12 9-10 10-11 11-12 21-22 27-28
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 8 :

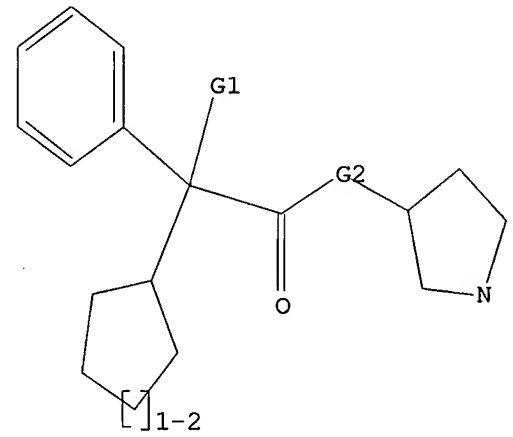
G1:O,N

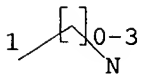
G2:O,N,[*1],[*2]

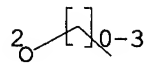
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 15:CLASS 16:CLASS 18:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 26:CLASS 27:CLASS 28:CLASS 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom

L6 STRUCTURE UPLOADED

=> d
L6 HAS NO ANSWERS
L6 STR







G1 O,N
G2 O,N,[@1],[@2]

Karen Cheng

10540245

Structure attributes must be viewed using STN Express query preparation.

=> s l6 full sub=l5
FULL SUBSET SEARCH INITIATED 14:51:39 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 257 TO ITERATE

100.0% PROCESSED 257 ITERATIONS 254 ANSWERS
SEARCH TIME: 00.00.01

L7 254 SEA SUB=L5 SSS FUL L6

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 41.10 386.38

FILE 'CAPLUS' ENTERED AT 14:51:49 ON 13 MAR 2007
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FILE COVERS 1907 - 13 Mar 2007 VOL 146 ISS 12
FILE LAST UPDATED: 11 Mar 2007 (20070311/ED)

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=> s l7
L8 350 L7

=> fil stng
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.47 386.85

FILE 'STNGUIDE' ENTERED AT 14:51:55 ON 13 MAR 2007
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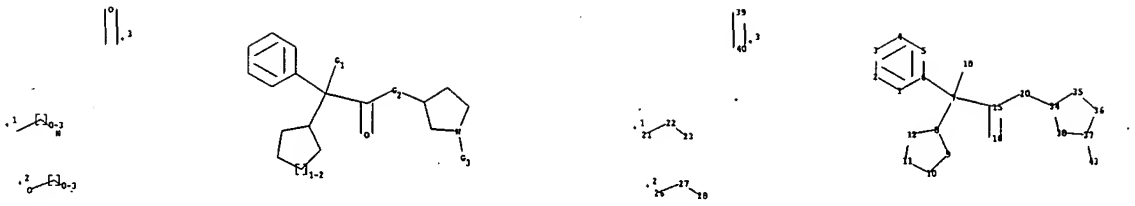
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 9, 2007 (20070309/UP).

=> fil reg

Karen Cheng



chain nodes :
7 15 16 18 20 21 22 23 26 27 28 39 40 43
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 34 35 36 37 38
chain bonds :
6-7 7-8 7-15 7-18 15-16 15-20 20-34 21-22 22-23 26-27 27-28 37-43 39-40

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 34-35 34-38 35-36
36-37 37-38
exact/norm bonds :
7-18 15-16 15-20 20-34 22-23 26-27 36-37 37-38 37-43 39-40
exact bonds :
6-7 7-8 7-15 8-9 8-12 9-10 10-11 11-12 21-22 27-28 34-35 34-38 35-36
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 8 : 34 :

G1:O,N

G2:O,N,[*1],[*2]

G3:C,S,[*3]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 15:CLASS 16:CLASS 18:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 26:CLASS 27:CLASS 28:CLASS 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom
39:CLASS 40:CLASS 43:CLASS

L9 STRUCTURE UPLOADED

Karen Cheng

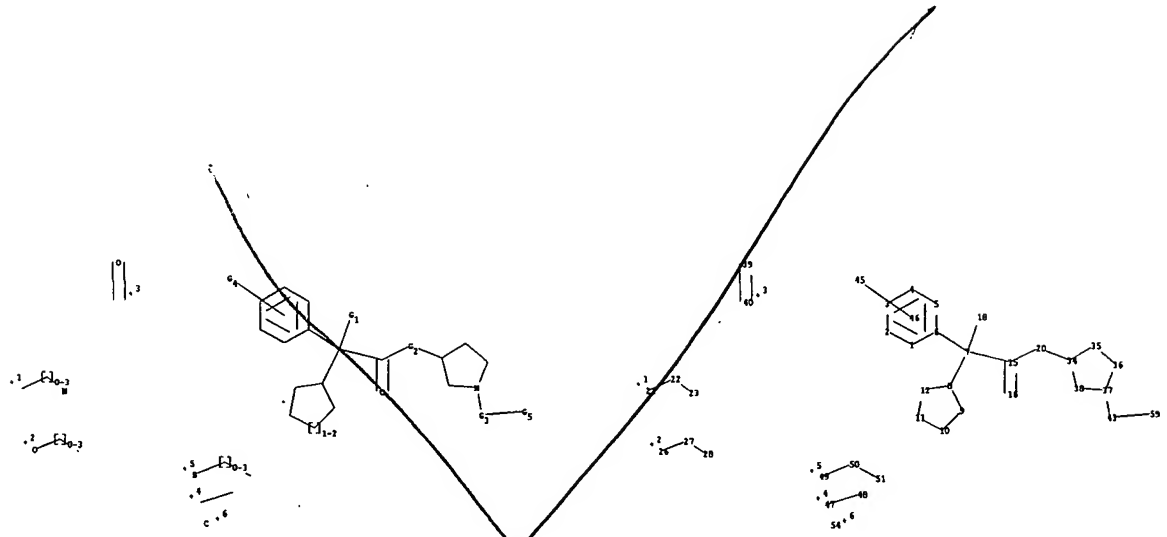
10540245

=> s l9 full sub=l7
FULL SUBSET SEARCH INITIATED 14:54:23 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 219 TO ITERATE

100.0% PROCESSED 219 ITERATIONS 216 ANSWERS
SEARCH TIME: 00.00.01

L10 216 SEA SUB=L7 SSS FUL L9

=>
Uploading C:\Program Files\Stnexp\Queries\10540245d.str



chain nodes :
7 15 16 18 20 21 22 23 26 27 28 39 40 43 45 47 48 49 50 51 54
59
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 34 35 36 37 38
chain bonds :
6-7 7-8 7-15 7-18 15-16 15-20 20-34 21-22 22-23 26-27 27-28 37-43 39-40
43-59 47-48 49-50 50-51
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 34-35 34-38 35-36
36-37 37-38
exact/norm bonds :
7-18 15-16 15-20 20-34 22-23 26-27 36-37 37-38 37-43 39-40 43-59 49-50
exact bonds :
6-7 7-8 7-15 8-9 8-12 9-10 10-11 11-12 21-22 27-28 34-35 34-38 35-36
47-48 50-51
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 8 : 34 :

Karen Cheng

10540245

G1:O,N

G2:O,N,[*1],[*2]

G3:C,S,[*3]

G4:H,X,Ak

G5:[*2],[*4],[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 15:CLASS 16:CLASS 18:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 26:CLASS 27:CLASS 28:CLASS 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom
39:CLASS 40:CLASS 43:CLASS 45:CLASS 46:Atom 47:CLASS 48:CLASS 49:CLASS
50:CLASS 51:CLASS 54:CLASS 59:CLASS

L11 STRUCTURE UPLOADED

=> d
L11 HAS NO ANSWERS
L11 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full sub=l10
FULL SUBSET SEARCH INITIATED 15:00:34 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.05

L12 0 SEA SUB=L10 SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\10540245e.str

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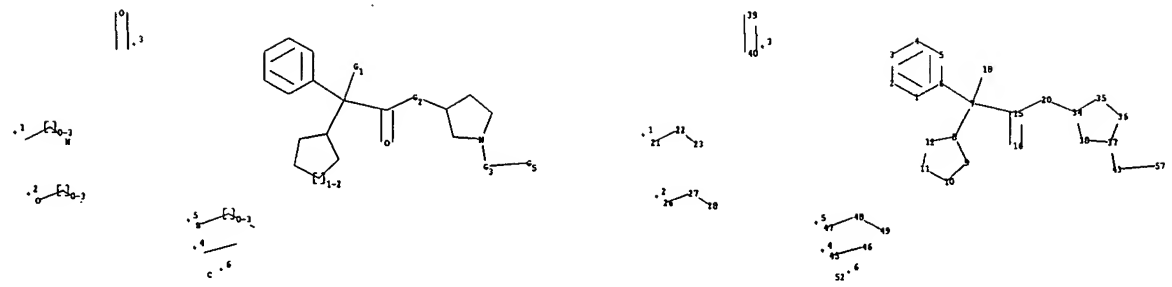

chain nodes :
7 15 16 18 20 21 22 23 26 27 28 39 40 43 45 46 47 48 49 52 57
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 34 35 36 37 38
chain bonds :
6-7 7-8 7-15 7-18 15-16 15-20 20-34 21-22 22-23 26-27 27-28 37-43 39-40
43-57 45-46 47-48 48-49
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 34-35 34-38 35-36
36-37 37-38
exact/norm bonds :
7-18 15-16 15-20 20-34 22-23 26-27 36-37 37-38 37-43 39-40 43-57 47-48
exact bonds :
6-7 7-8 7-15 8-9 8-12 9-10 10-11 11-12 21-22 27-28 34-35 34-38 35-36
45-46 48-49
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 8 : 34 :

G1:O,N

G2:O,N,[*1],[*2]

G3:C,S,[*3]

G4:H,X,Ak

G5:[*2],[*4],[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 15:CLASS 16:CLASS 18:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 26:CLASS 27:CLASS 28:CLASS 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom
39:CLASS 40:CLASS 43:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS
52:CLASS 57:CLASS

10540245

```
L13     STRUCTURE UPLOADED

=> d
L13 HAS NO ANSWERS
L13             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> d his

     (FILE 'HOME' ENTERED AT 14:45:22 ON 13 MAR 2007)

     FILE 'REGISTRY' ENTERED AT 14:45:29 ON 13 MAR 2007
L1              STRUCTURE UPLOADED
L2            0 S L1 FULL
L3              STRUCTURE UPLOADED
L4           50 S L3
L5         3003 S L3 FULL

     FILE 'STNGUIDE' ENTERED AT 14:47:06 ON 13 MAR 2007

     FILE 'REGISTRY' ENTERED AT 14:51:18 ON 13 MAR 2007
L6              STRUCTURE UPLOADED
L7          254 S L6 FULL  SUB=L5

     FILE 'CAPLUS' ENTERED AT 14:51:49 ON 13 MAR 2007
L8          350 S L7

     FILE 'STNGUIDE' ENTERED AT 14:51:55 ON 13 MAR 2007

     FILE 'REGISTRY' ENTERED AT 14:53:42 ON 13 MAR 2007
L9              STRUCTURE UPLOADED
L10         216 S L9 FULL  SUB=L7
L11             STRUCTURE UPLOADED
L12           0 S L1 FULL  SUB=L10
L13             STRUCTURE UPLOADED

=> s l13 full sub = l10
FULL SUBSET SEARCH INITIATED 15:01:52 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -      216 TO ITERATE

100.0% PROCESSED      216 ITERATIONS                              89 ANSWERS
SEARCH TIME: 00.00.01

L14          89 SEA SUB=L10 SSS FUL L13

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               128.25     515.28


Karen Cheng
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10540245

FILE 'CAPLUS' ENTERED AT 15:01:57 ON 13 MAR 2007
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FILE COVERS 1907 - 13 Mar 2007 VOL 146 ISS 12
FILE LAST UPDATED: 11 Mar 2007 (20070311/ED)

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http://www.cas.org/infopolicy.html

=> s l14
L15 12 L14

=> d ibib abs hitstr tot

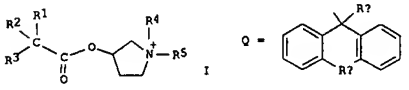
Karen Cheng

L15 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:633933 CAPLUS
DOCUMENT NUMBER: 145:103724
TITLE: Preparation of pyrrolidinium derivatives for treatment of conditions mediated by M3 muscarinic receptors
INVENTOR(S): Press, Neil John; Collingwood, Stephen Paul
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006066928	A1	20060629	WO 2005-EP13896	20051222

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: GB 2004-28416 A 20041224
OTHER SOURCE(S): MARPAT 145:103724
GI

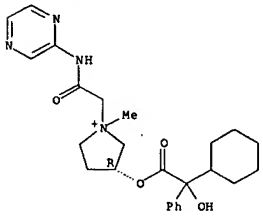


I

AB The title compds. I [R1, R3 = carbocyclic group, heterocyclic group having at least one ring heteroatom selected from N, O, and S; R2 = H, OH, alkyl optionally substituted by hydroxy; or CR1R2R3 = Q; Ra = bond, O, S, etc.; Rb = H, OH, alkyl optionally substituted by hydroxy; R4 = alkyl; R5 = C1 alkyl (substituted by CO2R6, CONHR6), C2 - C10 alkyl (substituted by OCOR6, etc.), etc.; R6 = C3 - C15 carbocyclic group, heterocyclic group (having at least one ring heteroatom selected from nitrogen, oxygen, sulfur), etc.] in salt or zwitterionic forms are prepared Thus, (1R/S,3R)-3-((R/S)-(2-cyclohexyl-2-hydroxy-2-phenylacetoxy))-1-methyl-1-(pyrazin-2-ylcarbamoylmethyl)pyrrolidinium bromide was prepared in several steps starting from aminopyrazine and bromoacetyl chloride. In an assay

L15 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
for the affinity for the human muscarinic acetylcholine M3 receptors, compds. of this invention have IC50 values below 1 μM.
IT 896125-47-6P 896125-48-7P 896125-49-8P
896125-50-1P 896125-51-2P 896125-52-3P
896125-59-0P 896125-60-3P 896125-61-4P
896125-62-5P 896125-63-6P 896125-64-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrrolidinium derivs. for treatment of conditions mediated
by M3 muscarinic receptors)
RN 896125-47-6 CAPLUS
CN Pyrrolidinium, 3-[(cyclohexylhydroxyphenylacetyl)oxy]-1-methyl-1-[2-oxo-2-(pyrazinylamino)ethyl]-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

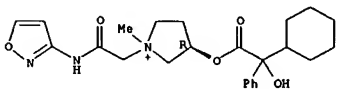


● Br⁻

RN 896125-48-7 CAPLUS
CN Pyrrolidinium, 3-[(cyclohexylhydroxyphenylacetyl)oxy]-1-[2-(3-isoxazolylamino)-2-oxoethyl]-1-methyl-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

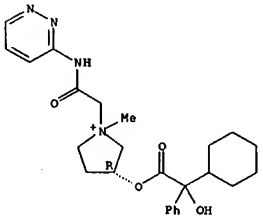
L15 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Br⁻

RN 896125-49-8 CAPLUS
CN Pyrrolidinium, 3-[(cyclohexylhydroxyphenylacetyl)oxy]-1-methyl-1-[2-oxo-2-(3-pyridazinylamino)ethyl]-, bromide, (3R)- (9CI) (CA INDEX NAME)

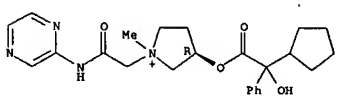
Absolute stereochemistry.



● Br⁻

RN 896125-50-1 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-methyl-1-[2-oxo-2-(pyrazinylamino)ethyl]-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

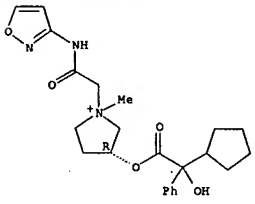


● Br⁻

L15 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 896125-51-2 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-[2-(3-isoxazolylamino)-2-oxoethyl]-1-methyl-, bromide, (3R)- (9CI) (CA INDEX NAME)

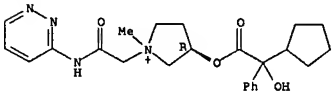
Absolute stereochemistry.



● Br⁻

RN 896125-52-3 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-methyl-1-[2-oxo-2-(3-pyridazinylamino)ethyl]-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

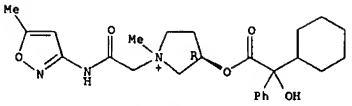


● Br⁻

RN 896125-59-0 CAPLUS
CN Pyrrolidinium, 3-[(cyclohexylhydroxyphenylacetyl)oxy]-1-methyl-1-[2-[(5-methyl-3-isoxazolyl)amino]-2-oxoethyl]-, (3R)- (9CI) (CA INDEX NAME)

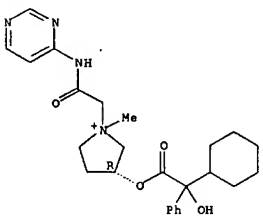
Absolute stereochemistry.

L15 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



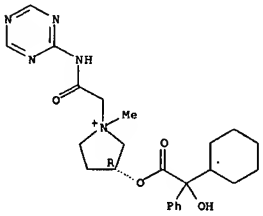
RN 896125-60-3 CAPLUS
CN Pyrrolidinium, 3-[(cyclohexylhydroxyphenylacetyl)oxy]-1-methyl-1-[2-oxo-2-(4-pyrimidinylamino)ethyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 896125-61-4 CAPLUS
CN Pyrrolidinium, 3-[(cyclohexylhydroxyphenylacetyl)oxy]-1-methyl-1-[2-oxo-2-(1,3,5-triazin-2-ylamino)ethyl]-, (3R)- (9CI) (CA INDEX NAME)

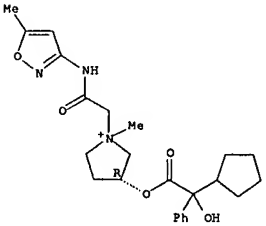
Absolute stereochemistry.



L15 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

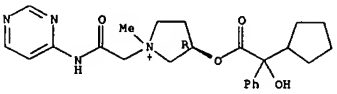
RN 896125-62-5 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-methyl-1-[2-[(5-methyl-3-isoxazolyl)amino]-2-oxoethyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



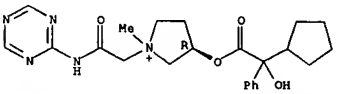
RN 896125-63-6 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-methyl-1-[2-oxo-2-(4-pyrimidinylamino)ethyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 896125-64-7 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-methyl-1-[2-oxo-2-(1,3,5-triazin-2-ylamino)ethyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L15 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

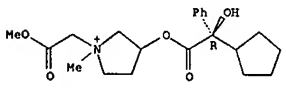
ACCESSION NUMBER: 2006:185956 CAPLUS
DOCUMENT NUMBER: 144:444887
TITLE: Pharmacological effects of some newly developed soft anticholinergics and a receptor-binding QSAR study
AUTHOR(S): Mori, N.; Buchwald, P.; Wu, W.-M.; Ji, F.; Hochhaus, G.; Bodor, N.
CORPORATE SOURCE: Center for Drug Discovery, University of Florida, FL, USA
SOURCE: Pharmazie (2006), 61(2), 148-153
CODEN: PHARAT; ISSN: 0031-7144
PUBLISHER: Govi-Verlag Pharmazeutischer Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Receptor-binding studies using cloned human muscarinic receptors (M1-M4 subtypes) were performed on newly synthesized soft anticholinergics (F-828, F-838, SGM, SGE, SA-A) that are isosteric/isoelectronic analogs of glycopyrrolate. The receptor binding pKi values of the new soft drugs were in the 5.5-9.5 range; with the majority being in the 7.0-8.5 range. As previously observed for similar structures, the pKi values tended to decrease with increasing mol. size, and with the introduction of three structural indicator variables, a QSAR equation accounting for close to 75% of the variability could be established. Confirming the known stereospecificity of these receptors, pure 2R isomers were found more active than the corresponding isomeric mixts. In agreement with soft drug design principles, acid metabolites (SA-A) were found considerably less active than their parent esters. The more active, 2R isomer of SA-A showed some muscarinic subtype selectivity (M3/M2), which was not observed for the parent compds. of this zwitterionic metabolite. Guinea pig ileum assay pA2 values have also been determined, and they were in good agreement with the pKi values obtained from the binding study (r^2 = 0.72). SGM and SGE caused pupil-dilation in rabbit eyes, but their mydriatic effects lasted considerably shorter than that of glycopyrrolate, and they did not induce dilation of the pupil in the contralateral, water-treated eyes, indicating that they are locally active and safe, with a low potential to cause systemic side effects.

IT 874098-41-6 874098-42-7 874098-43-8
874098-44-9 877845-96-0 877845-98-2
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacol. effects of soft anticholinergics and receptor-binding QSAR study)

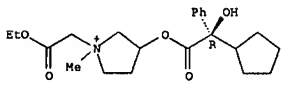
RN 874098-41-6 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-(2-methoxy-2-oxoethyl)-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

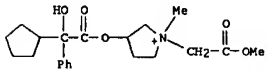


RN 874098-42-7 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-(2-ethoxy-2-oxoethyl)-1-methyl- (9CI) (CA INDEX NAME)

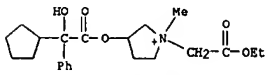
L15 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Absolute stereochemistry.



RN 874098-43-8 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-(2-methoxy-2-oxoethyl)-1-methyl- (9CI) (CA INDEX NAME)

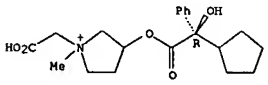


RN 874098-44-9 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-(2-ethoxy-2-oxoethyl)-1-methyl- (9CI) (CA INDEX NAME)



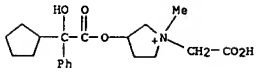
RN 877845-96-0 CAPLUS
CN Pyrrolidinium, 1-(carboxymethyl)-3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 877845-98-2 CAPLUS
CN Pyrrolidinium, 1-(carboxymethyl)-3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-methyl- (9CI) (CA INDEX NAME)

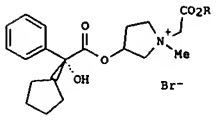
L15 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:185945 CAPLUS
DOCUMENT NUMBER: 145:210823
TITLE: Preparation and biological effects of pure stereoisomeric novel soft anticholinergics
AUTHOR(S): Toth-Sarudy, E.; Toth, G.; Pallagi, I.; Seres, G.; Vitalis, B.; Tapfer, M.; Perczel, V.; Kurucz, I.; Bodor, N.; Zubovics, Z.
CORPORATE SOURCE: IVAX Drug Research Institute Ltd, Budapest, Hung.
SOURCE: Pharmazie (2006), 61(2), 90-96
CODEN: PHARAT; ISSN: 0031-7144
PUBLISHER: Govi-Verlag Pharmazeutischer Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:210823
GI

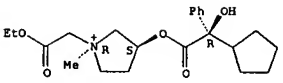


I

AB A series of pure stereoisomeric soft glycopyrrolate analogs I (R = Et, n-hexyl, n-octyl) was synthesized using chiral intermediates and by careful separation of the stereoisomers formed during the last quaternization step of the synthesis. The stereochem. of the products was elucidated using various 1D and 2D NMR techniques. Anticholinergic activity of the new compds. was determined by receptor binding studies and performing tests on isolated organs and by in vivo tests. Receptor binding revealed that in the higher alkyl ester series the (2R,1'R,3'R) and the (2R,1'S,3'S) isomers have showed the highest receptor affinity; furthermore, it demonstrated the confines of the length of the alkyl chain. In vitro isolated organ expts. correlated well with the receptor binding results, and in vivo investigations indicated the soft character of the compds.
IT 904673-14-9P 904673-15-0P 904673-16-1P
904673-17-2P 904673-18-3P 904673-19-4P
904673-20-7P 904673-21-8P 904673-22-9P
904673-23-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and biol. evaluation of stereoisomeric N-alkoxycarbonylmethyl (hydroxyacetoxy)pyrrolidinium bromides as soft anticholinergics)
RN 904673-14-9 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-(2-ethoxy-2-oxoethyl)-1-methyl-, bromide, (1R,3S)- (9CI) (CA INDEX NAME)

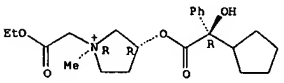
Absolute stereochemistry.

L15 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



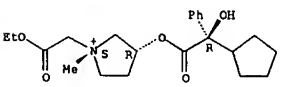
RN 904673-15-0 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-(2-ethoxy-2-oxoethyl)-1-methyl-, bromide, (1R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 904673-16-1 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-(2-ethoxy-2-oxoethyl)-1-methyl-, bromide, (1S,3R)- (9CI) (CA INDEX NAME)

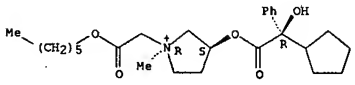
Absolute stereochemistry.



RN 904673-17-2 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-[2-(hexyloxy)-2-oxoethyl]-1-methyl-, bromide, (1R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

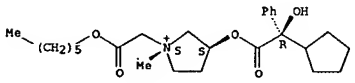
L15 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Br⁻

RN 904673-18-3 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-[2-(hexyloxy)-2-oxoethyl]-1-methyl-, bromide, (1S,3S)- (9CI) (CA INDEX NAME)

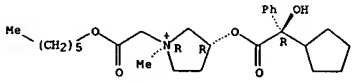
Absolute stereochemistry.



● Br⁻

RN 904673-19-4 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-[2-(hexyloxy)-2-oxoethyl]-1-methyl-, bromide, (1R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

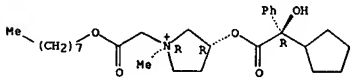


● Br⁻

RN 904673-20-7 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-[2-(hexyloxy)-2-oxoethyl]-1-methyl-, bromide, (1S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

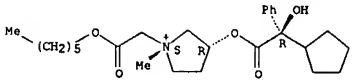
L15 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Br⁻

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

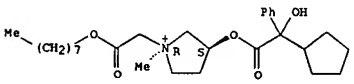
L15 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Br⁻

RN 904673-21-8 CAPLUS
CN Pyrrolidinium, 3-[[(cyclopentylhydroxyphenylacetyl)oxy]-1-methyl-1-[2-(octyloxy)-2-oxoethyl]-, bromide, (1R,3S)-rel- (9CI) (CA INDEX NAME)

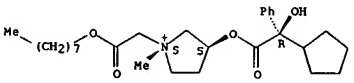
Relative stereochemistry.



● Br⁻

RN 904673-22-9 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-methyl-1-[2-(octyloxy)-2-oxoethyl]-, bromide, (1S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br⁻

RN 904673-23-0 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-methyl-1-[2-(octyloxy)-2-oxoethyl]-, bromide, (1R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L15 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

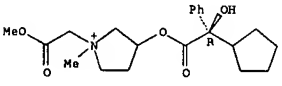
ACCESSION NUMBER: 2006:20539 CAPLUS
DOCUMENT NUMBER: 144:285622
TITLE: Soft Quaternary Anticholinergics: Comprehensive Quantitative Structure-Activity Relationship (QSAR) with a Linearized Biexponential (LinBiExp) Model
AUTHOR(S): Buchwald, Peter; Bodor, Nicholas
CORPORATE SOURCE: IVAX Research, Inc., Miami, FL, 33137, USA
SOURCE: Journal of Medicinal Chemistry (2006), 49(3), 883-891
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A comprehensive quant. structure-activity relationship (QSAR) study is presented for quaternary soft anticholinergics including two distinctly different classes designed on the basis of the soft analog and the inactive metabolite approaches. Because of the clear biphasic (bilinear) nature of the activity data when all structures (n = 76) were considered as a function of mol. size (volume), a nonlinear model had to be used, and a linearized biexponential (LinBiExp) model proved very adequate. LinBiExp can fit activity data that show a maximum (or a min.) around a given parameter value but tend to show linearity away from this turning point. Contrary to Hansch-type parabolic models, LinBiExp represents a natural extension of linear models, and a direct correspondence between its parameters and those obtained earlier by linear regression on compound subsets covering more limited parameter ranges could be easily established. Stereospecificity was confirmed as important, and the presence of an acid moiety was found to essentially eliminate activity. The consideration of bilinear behavior, which most likely results from size limitations at the binding site, can also explain the embarrassingly low activity found for a relatively large compound predicted as highly active by Lien at al. based on their QSAR study.

IT 874098-41-6 874098-42-7 874098-43-8
874098-44-9 877845-96-0 877845-98-2
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(comprehensive quant. structure-activity relationship (QSAR) with a linearized biexponential (LinBiExp) model for soft quaternary anticholinergics)

RN 874098-41-6 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-(2-methoxy-2-oxoethyl)-1-methyl- (9CI) (CA INDEX NAME)

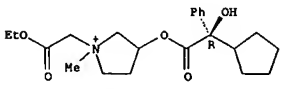
Absolute stereochemistry.



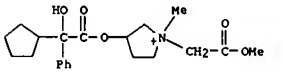
RN 874098-42-7 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-(2-ethoxy-2-oxoethyl)-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

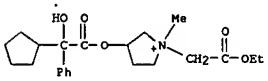
L15 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 874098-43-8 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-(2-methoxy-2-oxoethyl)-1-methyl- (9CI) (CA INDEX NAME)

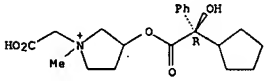


RN 874098-44-9 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-(2-ethoxy-2-oxoethyl)-1-methyl- (9CI) (CA INDEX NAME)



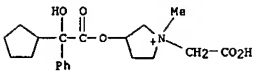
RN 877845-96-0 CAPLUS
CN Pyrrolidinium, 1-(carboxymethyl)-3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 877845-98-2 CAPLUS
CN Pyrrolidinium, 1-(carboxymethyl)-3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-methyl- (9CI) (CA INDEX NAME)

L15 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

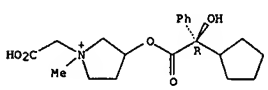
ACCESSION NUMBER: 2005:1335769 CAPLUS
DOCUMENT NUMBER: 144:267112
TITLE: Pharmacokinetic and Pharmacodynamic Evaluations of the Zwitterionic Metabolite of a New Series of N-Substituted Soft Anticholinergics
AUTHOR(S): Wu, Whei-Mei; Buchwald, Peter; Mori, Nobuhiro; Ji, Fubao; Wu, JiaXiang; Bodor, Nicholas
CORPORATE SOURCE: Center for Drug Discovery, College of Pharmacy, University of Florida, Gainesville, FL, USA
SOURCE: Pharmaceutical Research (2005), 22(12), 2035-2044
CODEN: PHREEB; ISSN: 0724-8741
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Purpose: This study was conducted to evaluate the zwitterionic common metabolite of a novel series of N-substituted soft analogs of glycopyrrolate both as racemates and as 2R isomers. Methods: Activities were assessed using both in vitro (receptor binding assay, guinea pig ileum pA2 assay) and in vivo techniques (rabbit mydriatic response, rat cardiac effects). Pharmacokinetic characterizations in rats were also performed. Results: The metabolite was highly water-soluble and very stable in buffer solns. as well as in rat biol. media. Following i.v. administration in rats, it was very rapidly eliminated, mainly through renal excretion with a half-life of about 10 min. Receptor binding and guinea pig ileum assays indicated this metabolite as more than 1 order of magnitude less active than its parent soft drugs or glycopyrrolate. Moderate M3/M2 muscarinic receptor subtype selectivity was observed, further reducing the likelihood of cardiac side effects. The metabolite showed to some extent mydriatic effect and protective effect against carbachol-induced bradycardia, but of much shorter durations than glycopyrrolate; it had, however, no effect on resting heart rate. Conclusions: N-Substituted zwitterionic metabolites retain some, but only considerably reduced activity of their parent quaternary ammonium ester soft anticholinergic drugs, and they are very rapidly eliminated from the systemic circulation. They are suitable for their assigned role within the framework of inactive metabolite-based soft anticholinergic design.

IT 877845-96-0
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacokinetic and pharmacodynamic evaluations of zwitterionic metabolite of a new series of N-Substituted soft anticholinergics)

RN 877845-96-0 CAPLUS
CN Pyrrolidinium, 1-(carboxymethyl)-3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

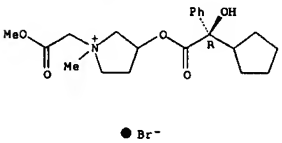


IT 873912-88-0 873912-89-1 877845-98-2
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

L15 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(pharmacokinetic and pharmacodynamic evaluations of zwitterionic metabolite of a new series of N-Substituted soft anticholinergics)

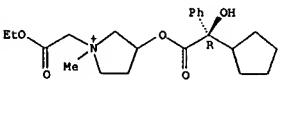
RN 873912-88-0 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-(2-methoxy-2-oxoethyl)-1-methyl-, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

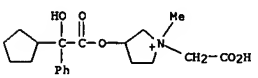


RN 873912-89-1 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-(2-ethoxy-2-oxoethyl)-1-methyl-, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 877845-98-2 CAPLUS
CN Pyrrolidinium, 1-(carboxymethyl)-3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Karen Cheng

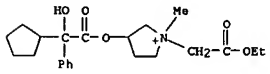
L15 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1274150 CAPLUS
DOCUMENT NUMBER: 144:141992
TITLE: Synthesis and pharmacological effects of new, N-substituted soft anticholinergics based on glycopyrrolate
AUTHOR(S): Ji, F.; Wu, W.; Dai, X.; Mori, N.; Wu, J.; Buchwald, P.; Bodor, N.
CORPORATE SOURCE: Center for Drug Discovery, College of Pharmacy, University of Florida, Gainesville, FL, 32610-0497, USA
SOURCE: Journal of Pharmacy and Pharmacology (2005), 57(11), 1427-1435
CODEN: JPPMAB; ISSN: 0022-3573
PUBLISHER: Pharmaceutical Press
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:141992

AB To reduce the possibility of systemic side-effects in locally administered anticholinergics, two new N-substituted glycopyrrolate analogs designed using soft drug design approaches have been synthesized and evaluated in vitro and in vivo. Because stereospecificity is known to be important at muscarinic receptors, the new compds. SGM and SGE also have been prepared as their pure 2R isomers, 2R-SGM and 2R-SGE, by starting from optically pure (-)-cyclopentylmandelic acid, and the corresponding isomers were indeed found to be more active. The new soft glycopyrrolates were chemical more stable under acidic conditions, and the Et esters SGE were more stable than the Me esters SGM. The new compds. were also found to be quite susceptible to extrahepatic metabolism, having half-lives of 20-30 min in rat plasma (in vitro), consistent with their soft nature. Binding studies at human muscarinic receptors (M1-M4) and guinea-pig ileum assays found 2R-SGM and 2R-SGE to have potencies somewhat less than, but close to, those of glycopyrrolate and N-methylscopolamine. They caused pupil dilation in rabbit eyes, but their mydriatic effects lasted for considerably less time than that of glycopyrrolate, and they did not induce dilation of the pupil in the contralateral, water-treated eyes, indicating that, in agreement with their soft nature, they are locally active, but safe and with a low potential to cause systemic side-effects.

IT 873912-88-0P 873912-89-1P 873912-90-4P
873912-91-5P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and pharmacol. effects of N-substituted soft anticholinergics based on glycopyrrolate)

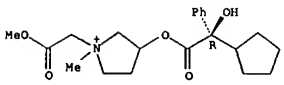
RN 873912-88-0 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-(2-methoxy-2-oxoethyl)-1-methyl-, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br⁻

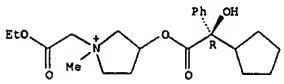
L15 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Br⁻

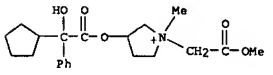
RN 873912-89-1 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-(2-ethoxy-2-oxoethyl)-1-methyl-, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br⁻

RN 873912-90-4 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-(2-methoxy-2-oxoethyl)-1-methyl-, bromide (9CI) (CA INDEX NAME)



● Br⁻

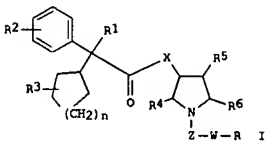
RN 873912-91-5 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-(2-ethoxy-2-oxoethyl)-1-methyl-, bromide (9CI) (CA INDEX NAME)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:546475 CAPLUS
DOCUMENT NUMBER: 141:106362
TITLE: Preparation of 1-substituted-3-pyrrolidine derivatives as muscarinic receptor antagonists
INVENTOR(S): Mehta, Anitar Gupta, Jang Bahadur; Sarma, Pakala Kumara Savithru
PATENT ASSIGNEE(S): Ranbaxy Laboratories Limited, India
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056767	A1	20040708	WO 2002-IB5590	20021223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002347552	A1	20040714	AU 2002-347552	20021223
EP 1583741	A1	20051012	EP 2002-783480	20021223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2006194862	A1	20060831	US 2006-540245	20060207
PRIORITY APPLN. INFO.:			WO 2002-IB5590 A	20021223

OTHER SOURCE(S): CASREACT 141:106362; MARPAT 141:106362
GI



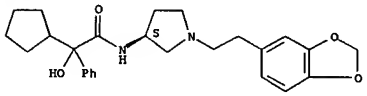
Current app

AB Title muscarinic receptor antagonists I (X = O, NH, etc.; R1 = OH, etc.; R2 = H, halo, alkyl; R3 = H, OH, etc.; R4, R5, R6 = H, alkyl; ; Z = CH2, SO2, carbonyl; W = alkylene, etc.; R = alkyl, aryl, etc.), useful for the treatment of various diseases of the respiratory, urinary and gastrointestinal systems mediated through muscarinic receptors, are prepared The affinity of these compds. for M2 and M3 muscarinic receptor subtype was tested. For example, (3S)-1-benzylpyrrolidin-3-yl

Karen Cheng

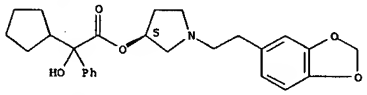
L15 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
cyclopentyl(hydroxy)phenylacetate was prepd. and had pKi = 6.13/7.17 for the M2 and M3 receptor subtype resp.
IT 719278-60-1P 719278-62-3P 719278-63-4P
719278-64-5P 719278-69-0P 719278-70-3P
719278-71-4P 719278-74-7P 719278-75-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-substituted-3-pyrrolidine derivs. as muscarinic receptor
antagonists)
RN 719278-60-1 CAPLUS
CN Benzeneacetamide, N-[(3S)-1-[2-(1,3-benzodioxol-5-yl)ethyl]-3-pyrrolidinyl]-α-cyclopentyl-α-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



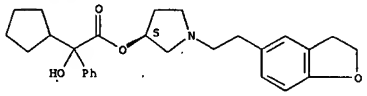
RN 719278-62-3 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[2-(1,3-benzodioxol-5-yl)ethyl]-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 719278-63-4 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[2-(2,3-dihydro-5-benzofuranyl)ethyl]-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

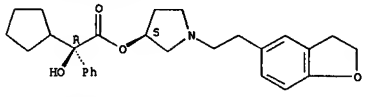
Absolute stereochemistry.



L15 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

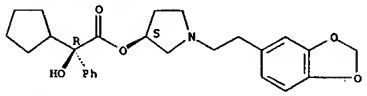
RN 719278-74-7 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[2-(2,3-dihydro-5-benzofuranyl)ethyl]-3-pyrrolidinyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 719278-75-8 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[2-(1,3-benzodioxol-5-yl)ethyl]-3-pyrrolidinyl ester, (αR)- (9CI) (CA INDEX NAME)

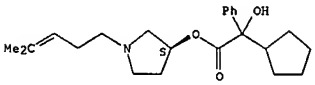
Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

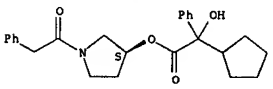
L15 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 719278-64-5 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-(4-methyl-3-pentenyl)-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



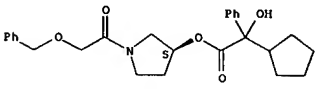
RN 719278-69-0 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-(phenylacetyl)-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



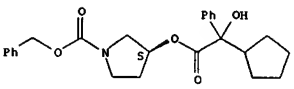
RN 719278-70-3 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[(phenylmethoxy)acetyl]-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 719278-71-4 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, 3-[[(cyclopentylhydroxyphenylacetyl)oxy]-, phenylmethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



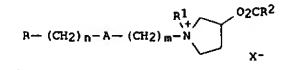
L15 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:837081 CAPLUS
DOCUMENT NUMBER: 139:337885
TITLE: Preparation of acyloxypyrrolidinium salts as M3 muscarinic antagonists
INVENTOR(S): Prat Quinones, Maria; Fernandez Forner, Maria Dolors
PATENT ASSIGNEE(S): Almirall Prodesfarma S.A., Spain
SOURCE: PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003087094	A2	20031023	WO 2003-EP3786	20030411
WO 2003087094	A3	20040318		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
ES 2206021	A1	20040501	ES 2002-889	20020416
ES 2206021	B1	20050801		
CA 2482536	A1	20031023	CA 2003-2482536	20030411
AU 2003233967	A1	20031027	AU 2003-233967	20030411
EP 1497284	A2	20050119	EP 2003-727294	20030411
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003009167	A	20050125	BR 2003-9167	20030411
CN 1662527	A	20050831	CN 2003-813892	20030411
ZA 2004008335	A	20051102	ZA 2004-8335	20041014
NO 2004004826	A	20050114	NO 2004-4826	20041105
US 2005282875	A1	20051222	US 2005-510680	20050720

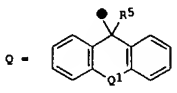
PRIORITY APPLN. INFO.: ES 2002-889 A 20020416
WO 2003-EP3786 W 20030411

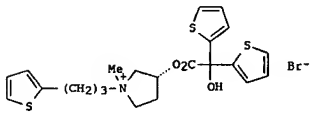
OTHER SOURCE(S): MARPAT 139:337885
GI

L15 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I





II

AB Pyrrolidinium derivs. I [R = (un)substituted Ph, naphthalenyl, 5,6,7,8-tetrahydronaphthalenyl, benzo[1,3]dioxolyl, biphenyl, heteroarom.; R1 = alkyl; R2 = CR3R4R5, Q; R3 = 2-furyl, 3-furyl, 2-thienyl, 3-thienyl; R4 = 2-furyl, 3-furyl, 2-thienyl, 3-thienyl, cycloalkyl; R5 = H, OH, Me, CH2OH; Q1 = CH2, CH2CH2, O, OCH2, S, SCH2, CH:CH; A = (un)substituted CH:CH, CH2, CO, O, S, S(O), SO2, NH; m = 0-8; n = 0-4] were prepared for use in therapy as antagonists of M3 muscarinic receptors (no data). Thus, (3R)-3-pyrrolidinol was treated with 2-(3-bromopropyl)thiophene to give (3R)-1-(3-thien-2-ylpropyl)pyrrolidinol which was treated with Me 2-hydroxy-2,2-dithen-2-ylacetate and quaternized to give the pyrrolidinium salt II.

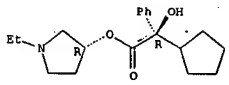
IT 616866-22-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of acyloxypyrrolidinium salts as M3 muscarinic antagonists)

RN 616866-22-9 CAPLUS

CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3R)-1-ethyl-3-pyrrolidinyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L15 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

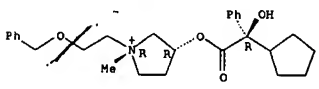


IT 616865-77-1P 616865-78-2P 616865-84-0P
616865-85-1P 616865-91-9P 616865-92-0P
616865-93-1P 616865-94-2P 616865-95-3P
616865-96-4P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of acyloxypyrrolidinium salts as M3 muscarinic antagonists)

RN 616865-77-1 CAPLUS

CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-methyl-1-[2-(phenylmethoxy)ethyl]-, bromide, (1R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

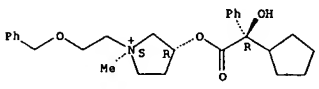


● Br⁻

RN 616865-78-2 CAPLUS

CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-methyl-1-[2-(phenylmethoxy)ethyl]-, bromide, (1S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



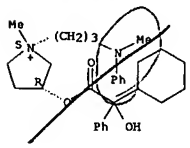
● Br⁻

RN 616865-84-0 CAPLUS

CN Pyrrolidinium, 3-[[(cyclohexylhydroxyphenylacetyl)oxy]-1-methyl-1-[3-(methylphenylamino)propyl]-, chloride, (1S,3R)- (9CI) (CA INDEX NAME)

L15 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry.

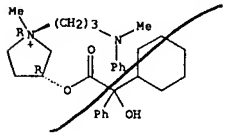


● Cl⁻

RN 616865-85-1 CAPLUS

CN Pyrrolidinium, 3-[(cyclohexylhydroxyphenylacetyl)oxy]-1-methyl-1-[3-(methylphenylamino)propyl]-, chloride, (1R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

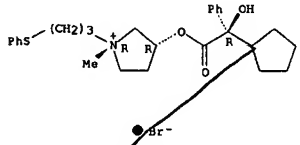


● Cl⁻

RN 616865-91-9 CAPLUS

CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-methyl-1-[3-(phenylthio)propyl]-, bromide, (1R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br⁻

RN 616865-92-0 CAPLUS

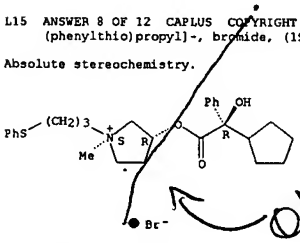
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-methyl-1-[3-

Karen Cheng

L15 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

(phenylthio)propyl]-, bromide, (1S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



Z = methylene.

W =

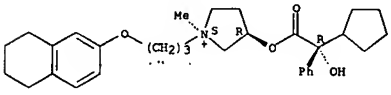
Okay.

● Br⁻

RN 616865-93-1 CAPLUS

CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-methyl-1-[3-[(5,6,7,8-tetrahydro-2-naphthalenyl)oxy]propyl]-, bromide, (1S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

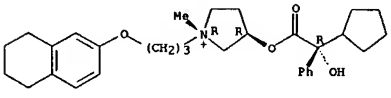


● Br⁻

RN 616865-94-2 CAPLUS

CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-methyl-1-[3-[(5,6,7,8-tetrahydro-2-naphthalenyl)oxy]propyl]-, bromide, (1R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



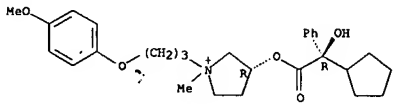
● Br⁻

RN 616865-95-3 CAPLUS

CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-[3-(4-methoxyphenoxy)propyl]-1-methyl-, bromide, (3R)- (9CI) (CA INDEX NAME)

L15 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

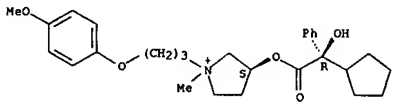
Absolute stereochemistry.



● Br⁻

RN 616865-96-4 CAPLUS
CN Pyrrolidinium, 3-[[(2R)-cyclopentylhydroxyphenylacetyl]oxy]-1-[3-(4-methoxyphenoxy)propyl]-1-methyl-, bromide, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



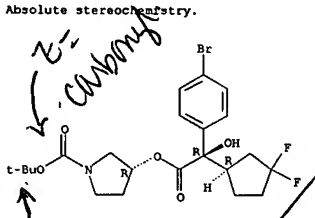
● Br⁻

L15 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
and sodium cyanoborohydride in the presence of ZnCl2 in MeOH at room temp. for 30 min gave 1-methylpiperidin-4-yl (2R)-((1R)-3,3-difluoropentyl)-2-hydroxy-2-phenylethanoate which was quaternized by Me bromide in MeCN at room temp. for 15 h to give 4-[[(2R)-2-((1R)-3,3-difluorocyclopentyl)-2-hydroxy-2-phenylethanoyl]oxy]-1,1-dimethylpiperidinium bromide (I). In a muscarinic receptor M2 and M3 antagonism assay, 4-(((2R)-2-((1R)-3,3-difluorocyclopentyl)-2-hydroxy-2-phenylethanoyl)oxy)-1,1-dimethylpiperidinium bromide in vitro exhibited KB of 9.6 nM for inhibiting the carbachol-induced redn. in heart beat in rat right atrium (muscarinic receptor M2 receptor) and that of 0.004 nM for inhibiting the carbachol-induced contraction of trachea (muscarinic receptor M3 receptor) with M2/M3 receptor ratio of 218. An ampule or a powder inhalation formulation contg. I were described.

IT 389890-48-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylhydroxyacetic acid ester derivs. as muscarinic M3 receptor antagonists for therapeutic agents)

RN 389890-48-6 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, 3-[[(2R)-(4-bromophenyl)[(1R)-3,3-difluorocyclopentyl]hydroxyacetyl]oxy]-, 1,1-dimethylethyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:51415 CAPLUS
DOCUMENT NUMBER: 136:118468
TITLE: Preparation of 2-aryl-2-hydroxyacetic acid ester derivatives as muscarinic M3 receptor antagonists
INVENTOR(S): Ogino, Yoshio; Kurihara, Hideki; Matsuda, Kenji; Numazawa, Tomoshige; Otake, Norikazu; Noguchi, Kazuhito
PATENT ASSIGNEE(S): Banyu Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 138 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004402	A1	20020117	WO 2001-JP5987	20010710
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001071027	A5	20020121	AU 2001-71027	20010710
CA 2415468	A1	20030110	CA 2001-2415468	20010710
EP 1302458	A1	20030416	EP 2001-949925	20010710
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003191316	A1	20031009	US 2003-332617	20030110
US 6846835	B2	20050125		
US 2005065211	A1	20050324	US 2004-983613	20041109
PRIORITY APPLN. INFO.:			JP 2000-210591 A	20000711
			WO 2001-JP5987 W	20010710
			US 2003-332617 A3	20030110

OTHER SOURCE(S): MARPAT 136:118468
AB Compds. of the general formula ArC(OH)(R1)CO2A [wherein A is a group of the general formula -B1-N+R2R3R4.X- or -B2-NR5CR6:NR7; Ar is aryl or heteroaryl, any of which may be substituted; B1 and B2 are each an aliphatic hydrocarbon group; R1 is fluorinated cycloalkyl; R2, R3 and R4 are each lower alkyl, or a single bond or alkylene, any of which is bonded to B1, or alternatively R2 and R3 may be united to form alkylene; R5 and R7 are each hydrogen, lower alkyl, or a single bond or alkylene, any of which is bonded to B2; R6 is hydrogen, lower alkyl, or N(R8)R9; R8 and R9 are independently hydrogen or lower alkyl; and X- is an anion] are prepared Thses compds. exhibit selective muscarinic M3 receptor antagonism with little side effects and are suitable for administration by inhalation and useful as therapeutic agents for respiratory system diseases including chronic obstructive pulmonary diseases, chronic bronchitis, asthma, chronic airway obstruction, pulmonary fibrosis, pulmonary emphysema, or rhinitis. Thus, reductive methylation of piperidin-4-yl (2R)-((1R)-3,3-difluoropentyl)-2-hydroxy-2-phenylethanoate by formaldehyde

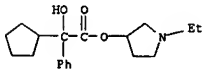
L15 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1963:469072 CAPLUS
DOCUMENT NUMBER: 59:69072
ORIGINAL REFERENCE NO.: 59:12765h,12766a-b
TITLE: 3-Pyrrolidyl glycolates
INVENTOR(S): Biel, John H.
PATENT ASSIGNEE(S): Lakeside Laboratories, Inc.
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3091570		19630528	US 1960-47897	19600808
PRIORITY APPLN. INFO.:			US	19600808

GI For diagram(s), see printed CA Issue.
AB The title compds., powerful antispasmodic and antisecretory agents and powerful stimulants of the central nervous system, may be prepared by treating a N-substituted 3-pyrrolidinol with a lower alkyl ester of a glycolic acid to form, via ester interchange, a 3-pyrrolidyl glycolate. Thus, 0.073 moles Me phenylcyclopentylglycolate (I), 0.073 mole N-methyl-3-pyrrolidinol, 0.5 g. NaOMe, and 200 ml. C7H16 was refluxed 5 hrs., as 4.3 ml. MeOH was collected. The mixture was filtered and the filtrate was washed with H2O, dried (K2CO3), and concentrated to dryness in vacuo to give 90.7% N-methyl-3-pyrrolidyl phenylcyclopentylglycolate (II); HCl salt m. 164-6° (MeCN). Similarly prepared from I and N-ethyl-3-hydroxypyrrolidine was 92% N-ethyl-3-pyrrolidyl phenylcyclopentylglycolate; HCl salt m. 105-6° (decomposition) (MeCN).

IT 60573-74-2P, Mandelic acid, α-cyclopentyl-, 1-ethyl-3-pyrrolidinyl ester, hydrochloride
RL: PREP (Preparation)
(preparation of)

RN 60573-74-2 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, 1-ethyl-3-pyrrolidinyl ester, hydrochloride (9CI) (CA INDEX NAME)



● HCl

Make this.

W= lower alkoxy

R= alkyl

X=oxo

R₁= hydroxy

n=1

R₃= fluoro

Karen Cheng

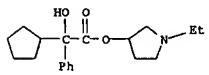
L15 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:69776 CAPLUS
DOCUMENT NUMBER: 56:69776
ORIGINAL REFERENCE NO.: 56:13402f-h
TITLE: Cholinergic blockade as an approach to the development of new psychotropic agents
AUTHOR(S): Biel, John H.; Nuhfer, Patrick A.; Hoya, Wallace K.; Leiser, Helen A.; Abood, Leo G.
CORPORATE SOURCE: Lakeside Labs., Inc., Milwaukee, WI
SOURCE: Annals of the New York Academy of Sciences (1962), 96, 251-62
CODEN: ANYAA9; ISSN: 0077-8923
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Tetrahydroaminacrine reversed the psychotic episode caused by an anticholinergic psychotogen. Only piperidyl and pyrrolidinyl esters exerted a great stimulation on the central nervous system. Ditran was an effective antidepressant. The largest concentration of these agents appeared, in
H3-labeled studies, in the hypothalamus and caudate nucleus of the brain, which controls mood and emotion.

IT 95423-66-8, Mandelic acid, α-cyclopentyl-, 1-ethyl-3-pyrrolidinyl ester
(parasympatholytic activity of)

RN 95423-66-8 CAPLUS

CN Mandelic acid, α-cyclopentyl-, 1-ethyl-3-pyrrolidinyl ester (6CI, 7CI) (CA INDEX NAME)



L15 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:60533 CAPLUS
DOCUMENT NUMBER: 56:60533
ORIGINAL REFERENCE NO.: 56:11557h-i,11558a-i,11559a-h
TITLE: Central stimulants. II. Cholinergic blocking agents
AUTHOR(S): Biel, John H.; Abood, Leo G.; Hoya, Wallace K.; Leiser, Helen A.; Nuhfer, Patrick A.; Kluchesky, E. F.
CORPORATE SOURCE: Lakeside Labs., Milwaukee, WI, USA
SOURCE: Journal of Organic Chemistry (1961), 26, 4096-103
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB cf. CA 48, 694a.--The initial finding that certain disubstituted glycolates of 3-hydroxypiperidine (I) could elicit potent psychotomimetic and antidepressant effects in man suggested a possible relationship between cholinergic blockade and central nervous system stimulatory properties. To investigate this hypothesis, a structural variety of esters of the hydroxypiperidines, hydroxypyrrolidines, and hydroxymethylpyrrolidines was synthesized. The following aspects of this investigation was discussed: (1) the ring contraction obtained during the reaction of the 3-halopiperidines with the free acid; (2) the thermal ring expansion during the distillation of the basic esters; (3) the structure activity relationships with regard to (a) central nervous system stimulation, (b) anticholinergic effects, and (c) the correlation of psychopharmacologic action with cholinergic blockade; (4) the use of these psychotogenic drugs as possible tools in the development of potential antagonists. At present, the conclusion appeared warranted that potent anticholinergic properties were a pharmacol. prerequisite for the characteristic central nervous system effects evoked by this group of compds. The assay method for the isomer ratio of N-ethyl-3-piperidyl phenylcyclopentylglyeolate (II) and N-ethyl-2-pyrrolidyhnethyl phenyleyclopentylglycolate (III) involved an acid hydrolysis of the esters, the extraction of the resulting alcs., and infrared spectrophotometric
determination of the ratio of the resulting alcs. Pure samples of N-ethyl-3-hydroxypiperidine (IV) and N-ethyl-2-hydroxymethylpyrrolidine (V) were prepared and infrared spectra taken. Standard mixts, were prepared from IV and V and the absorbance ratio plotted against % pyrrolidyl isomer and given in a figure. Samples of II and III were prepared by ester interchange using pure IV and V. Subsequent hydrolysis of II and III afforded alc. fragments with infrared spectra identical with that of starting materials. Thus, ring contraction did not occur during the esterification of the halopiperidine, resulting in a mixture of isomers. The procedure for the assay was described. N-Ethyl-3-chloropiperidine (VI) and 34.2 g. benzilic acid in 400 ml. iso-PrOH refluxed 12 hrs., evaporated, the residue taken up in H2O, made alkaline, the organic phase extracted with
Et2O, dried, evaporated, and the basic ether residue convetted to the HCl salt
in iso-PrOH gave 33 g. solids containing 55% N-ethyl-3-piperidyl benzilate-HCl
(VII), m. 163-7° (iso-PrOH). The mother liquor from the recrystn. was set aside to give mother liquor A for part B of the experiment The solid
recrystd. gave 12.5 g. pure VII, m. 191-2° (alc.). The mother

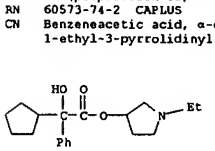
L15 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
liquor A concd. to one-fourth gave 12.5 g. N-ethyl-2pyrrolidylmethyl benzilate-HCl (VIII), m. 145-7°. Phenyl-cyclopentylglycolic acid (108.9 g.), 81.1 g. VI, and 625 cc. iso-PrOH refluxed 40 hrs., concd. to dryness, the residue dissolved in 1 l. H2O, extd. with Et2O, satd. with NaHCO3 soln., and the combined ether extd. dried, and evapd. The residue in 500 ml. Me2CO treated with Et2O-HCl gave 111.5 g. mixt. A 91.5 g. sample recrystd. gave 52 g. VII. The average isomer ratio from various expts. of VIII versus VII was found to be 70:30 as detd. by infrared spectroscopy. The filtrate gave 35.3 g. residue, m. 177-8°. The isomer ratio was the same as for the higher-melting material. The lower m.p. may be due to a different diastereoisomeric mixt. Me phenylcyclopentylglyeolate (106 g.), 64.5 g. N-ethyl-3hydroxypiperidine (IX), 1.5 g. NaOMe, and 1.26 l. heptane refluxed, the catalyst removed by filtration, the filtrate washed, the org. phase dried, evapd., and the 136.5 g. residue treated with Et2O-HCl gave 88 g. N-ethyl-3-piperidyl phenyleyclopentylgiycolate-HCl (X), m. 214-16° (isoPrOH). X by infrared spectrum was pure. A 70:30 mixt. of VII-VIII (55 g.) converted to the free base esters with aq. NaHCO3, extd. with Et2O, evapd., and the high-boiling ester distd. in vacuo gave 45 g. product, b0.05, 166-8°. Conversion of the base to the HCl salt gave the high-melting stereoisomer, m. 232-3°. The filtrate afforded 22% X. In subsequent runs this yield was as high as 40%. KOH (5.6 g.), 10.1 g. 2-pyrrolidyhnethanol, 11 g. EtBr, and 100 cc. alc. heated 2 hrs. at 100° in a pressure bottle gave 9 g. N-ethyl-2-pyrrolidylmethanol (XI), b2 8 50-1°. XI (10.6 g.), 19.3 g. Me phenylcyclopentylglycolate, 1 g. NaOMe, and 200 cc. heptane refluxed 4 hrs., the filtrate washed, dried, steam distd., and the 23.7 g. product acidified with HCl in Et2O gave 21.3 g. N-ethyl-2-pyrrolidylmethyl phenylcyclopentylglycolate-HCl (XII), m. 185-6° (MeCN). XII was shown by infrared assay to be pure. 3-Hydroxypiperidine (XIII) (65 g.) and 150 cc. PhMe refluxed 6 hrs. with 56.5 g. β-benzyloxyethyl chloride, the solid collected, the filtrate concd., and the product distd. gave 60 g. N-(βbenzyloxyethyl)-3-hydroxypiperidine (XIV), b1.1 150°, n25D 1.5321. XIV (38.8 g.), 36.3 g. Me benzilate, 0.6 g. NaOMe, and 400 cc. heptane refluxed, evapd., and the 67 g. product in Me2CO treated with HCl gave 50 g. N-(β-benzyloxyethyl)3-piperidyl benzilate-HCl (XV), m. 172° (MeOH). XV (24.1 g.), 3 g. Pd-C, and 150 cc. MeOH reduced at 60 lb./sq. in. at 25° gave 18.2 g. N-(β-hydroxyethyl)-3-piperidyl henzilate-HCl, m. 150-1°. N-Benzyl-3-piperidyl benzilate (20°g.), 3 g. AcOH, 3.5 g. 10% Pd-C, and 200 ml. MeOH reduced at 25° at 60 lb./sq. in. H pressure and acidified gave 16.8 g. 3-piperidyl benzilate-HCl, m. 178-80° NaOH (14.3 g.), 36 g. XIII, and 300 cc. 90% alc. refluxed 3 hrs. with 42 g.β-(4-methylpiperazino)ethyl chloride-HCl gave 16.3 g. 1- [β-(3-hydroxypiperidino) ethyl] 4-methylpiperazine, b0.6 120-2°, n25D 1.5061. XIII (101.4 g.) in 500 cc. C6H6 refuxed 4 hrs. with 53.8 g. β-dimethylaminoethyl chloride gave 73.2 g. N-(β-dimethylaminoethyl)-3-hydroxypiperidine, b0.9 92-4°, n25D 1.4822. XIII (68 g.), 67 g. NEt3, 132 g. a-bromoacetal, and 400 cc. PhMe refluxed 4 hrs., the HBr salt removed, the filtrate washed, and distd. gave 91 g. a-(3-hydroxypiperidino)acetal (XVI), b0.6 98-100°, n25D 1.4632. XVI (32.6 g.) left 3 hrs. at 25° under N with 75 cc. concd. HCl, evapd., the residue dild. with 150 cc. H2O, neutralized, treated overnight at 25° with 17.5 g. 1-amino-4methylpiperazine, the oil extd. with tetrahydrofuran, and concd. gave 32.4 g. crude hydrazone (XVII). XVII in 100 cc. tetrahydrofuran refluxed 4 hrs. with 5.2 g. LiAlH4 gave 23.7 g. 1-methyl-4-[β(2-hydroxypiperidino)ethylamino]piperazine, b0.03 147-9°. XIII (50.5 g.) and 50.5 g. H2O with 128 g. 30% H2SO4 treated during I hr. with 85 g. NaNO2 and 150 cc. H2O, the soln. stirred 1

L15 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
hr. at 25°, the oily layer extd. with CHCl3, the combined exts. washed with 40% KOH, and evapd. gave 40.9 g. N-nitroso-3-hydroxypiperidine (XVIII). XVIII (40.9 g.) in 300 cc. tetrahydrofuran treated in 1.5 hrs. with 17.5 g. LiAlH4 in 500 cc. tetrahydrofuran, the mixt. refluxed 1 hr., decompd., and the product distd. gave 25.9 g. 1-amino-3-hydroxypiperidine(XIX),b0.45 84-6°. XIX(60g.) and 38.5 g. Et formate refluxed 5 hrs., and the product distd. gave 41.5 g. N-formylamino-3-hydroxypiperidine (XIXa), b1.2 165°. XIXa (40.3 g.) and 250 cc. tetrahydrofuran added in 1.5 hrs. to 13.3 g. LiAlH4 in 500 cc. tetrahydrofuran, refluxed 3 hrs., decompd. with 40 cc. 40% aq. KOH, the salts removed, and the product distd. gave 25.9 g. N-methylamino-3-hydroxypiperidine, b1.2 83-6°, n25D 1.4972. XIII (50 g.), 50 g. NEt3, 62.5 g. PhCH2Cl, and 250 cc. PhMe refluxed 4 hrs. and the product distd. gave 65 g. Nbenzyl-4-hydroxypiperidine, b0.7 122-3°, n25D 1.5514. The following XX.HCl were prepd. (C5H9 = cyclopentyl) (R, R1, R2, ring position, Y, % yield, m.p. given): Et, Ph, C5H9, 3, --, --, --, 212-13° Me, C6H11, Ph, 3, --, 76, 222° H, Ph, Ph, 3, --, --, 96.5, 178-80° PhCH2, Ph, Ph, 3, --, 75.0, 222-3° Me2NCH2CH2, Ph, Ph, 3, --, 68.0, 237-8° PhCH2OCH2CH2, Ph, Ph, 3, --, 69, 172° PhCH2, Ph, Ph, 2, CH2, 67.2,211° HOCH2CH2, Ph, Ph, 3, --, 98.5, 1522.5° H, Ph, Ph, 2, CH2, 81, 199-200° Me, Ph, Ph, 2, CH2, 44.3,230° PhCH2, Ph, Ph, 4, --, 78.2, 194-5° Me, Ph, Ph, 2, CHCH3, 31.4, 230° H, Ph, Ph, 4, --, 88, 1802° Me, C5H9, Ph, 3, --, 58.7, 209-10° Et, Ph, C5H9, 4, --, 43.5, 220-1°; Me, Ph, Ph, 4, --, --, 213-14° Me, Ph, Ph, 2, CH2CH2, 26.7, 145-7° MeNH, Ph, Ph, 3, --, 30.0, 158-60° Me, Ph, Ph, 4, --, 53, 215-16°. The following XXIII.HCl were prepd. (R, R1, R2, ring position, Y, % yield, m.p. given): Et, Ph, C5H9, 2, CH2, 30, 186° Me, Ph, C5H9, 3, --, 31, 169-70° Et, Ph, C5H9, 3, --, 42, 165-6°. The following compds. were prepd. (% yield and m.p. given): 3-pyridylmethyl benzilate, 29.2,189° N-methyl-3piperidyl methyldiphenylacetate, 71, 216-17° 3-piperidyl diphenylacetate, 56.0, 171-2° XXI, 53, 257° XXII, 77, 237-9°. The central nervous system stimulation and E.D.50 values were given in a table for 36 compds. of the above types.

IT 60573-74-2P, 3-Pyrrolidinol, 1-ethyl-, α-cyclopentylmandelate, hydrochloride
RL: PREP (Preparation)
(preparation of)

RN 60573-74-2 CAPLUS

CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, 1-ethyl-3-pyrrolidinyl ester, hydrochloride (9CI) (CA INDEX NAME)



● HCl

The N-alkylation or carbonylation or sulphonylation of the compound of Formula V to give a compound of Formula I can be carried out in a suitable solvent such as N, N-dimethylformamide, dimethylsulfoxide, tetrahydrofuran, acetonitrile and dichloromethane.

In the above scheme, where specific bases, coupling agents, protecting groups, deprotecting agents, N-alkylating, sulphonylating, cabonylating agents, solvents, catalysts etc. are mentioned, it is to be understood that other bases, coupling agents deprotecting agents, N-alkylating, sulphonylating, carbonylating agents, solvents etc. known to those skilled in art may be used. Similarly, the reaction temperature and duration may be adjusted according to the desired needs.

The pharmaceutically acceptable salts of the compounds of Formula I include acid addition salts such as hydrochloride, hydrobromide, hydrofluoric, sulphate, bisulfate, phosphate, hydrogen phosphate, acetate, brosylate, citrate, fumarate, glyconate, lactate, maleate, mesylate, succinate, and tartarate.

Quaternary ammonium salts such as alkyl salts, aralkyl salts, and the like, of the organic bases may be readily formed by treatment of the organic bases with the appropriate quaternary salts forming substances, which include, for example methyl chloride, methyl bromide, methyl iodide, methyl sulphate, methyl benzene sulphonate, methyl p-toluene sulphonate, ethyl chloride, ethyl bromide, ethyl iodide, n-propyl chloride, n-propyl bromide, n-propyl iodide, isopropyl bromide, n-butyl chloride, n-butyl bromide, isobutyl bromide, sec-butylbromide, n-amyl bromide, n-hexyl chloride, benzyl chloride, benzyl bromide, and ethyl sulphate.

Particular compounds which are capable of being produced by Scheme I and shown in Table I include:

Compound No.	Chemical Name
1.	2-cyclopentyl-2-hydroxy-N-[(3S)-1-benzyl-pyrrolidin-3-yl]-2-phenyl acetamide
2.	2-cyclopentyl-2-hydroxy-N-[(3S)-1-[2-(1,3-benzodioxol-5-yl)]-ethyl]pyrrolidin-3-yl]-2-phenyl acetamide

3. (3S)-1-benzylpyrrolidin-3-yl cyclopentyl(hydroxy)phenyl acetate

4. (3S)-1-[[2-(1,3-benzodioxol-yl)ethyl]pyrrolidin-3yl]cyclopentyl(hydroxy)phenyl acetate

5. (3S)-1-[[2-(2,3-dihydro-1-benzofuran-5-yl)ethyl]pyrrolidin-3-yl]cyclopentyl-(hydroxy)phenyl acetate

6. (3S)-1-[(4-methyl-pent-3-enyl)pyrrolidin-3-yl] cyclopentyl(hydroxy)phenyl acetate

7. (3S)-1-[(4-trifluoromethylphenyl)sulfonyl]pyrrolidin-3-yl]cyclopentyl(hydroxy) phenyl acetate

8. (3S)-1-[(4-nitrophenyl]sulfonyl]pyrrolidin-3-yl]cyclopentyl(hydroxy)phenyl acetate

9. (3S)-1-benzyl-pyrrolidin-3-yl (2R)-hydroxy(3-oxocyclopentyl)phenyl acetate

10. (3S)-1-benzylpyrrolidin-3-yl (2R)-hydroxy(3-hydroxycyclopentyl)phenyl acetate

11. (3S)-1-[(phenylacetyl)pyrrolidin-3-yl] cyclopentyl(hydroxy)phenyl acetate

12. (3S)-1-[(benzyloxy)acetyl)pyrrolidin-3-yl]cyclopentyl(hydroxy)phenyl acetate

13. Benzyl (3S)-3-[(2-hydroxy-2-cyclopentyl-2-phenylpropanoyl)oxy]pyrrolidin-1-carboxylate

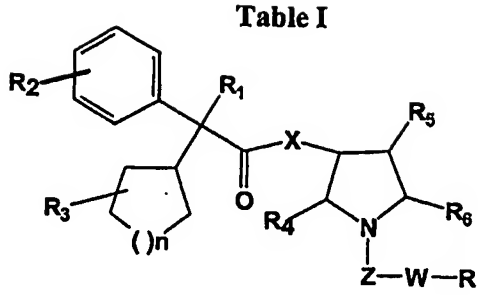
14. (3S)-1-[(4-bromophenyl)sulfonyl]pyrrolidin-3-yl]cyclopentyl(hydroxy)phenyl acetate

15. (3S)-1-benzylpyrrolidin-3-yl (2R)-cyclopentyl(hydroxy)phenyl acetate

16. (3S)-1-[[2-(2,3-dihydro-1-benzofuran-5-yl)ethyl]pyrrolidin-3-yl] (2R)cyclopentyl(hydroxy)phenyl acetate

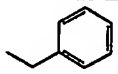
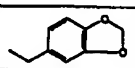
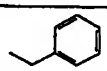
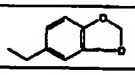
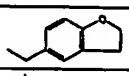
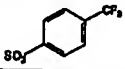
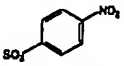
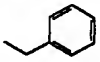
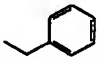
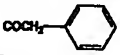
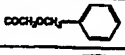
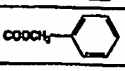
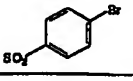
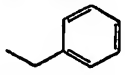
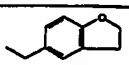
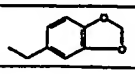
17. (3S)-1-[[2-(1,3-benzodioxol-5-yl)ethyl]pyrrolidin-3-yl (2R)-cyclopentyl(hydroxy) phenyl acetate

Table I

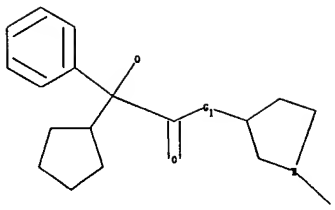


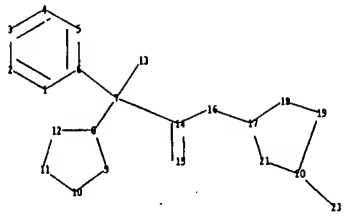
Formula I

(wherein R_1=OH, R_2=R_4=R_5=R_6=H, n=1)

Compound No.	Z-W-R	X	R_3	Configuration at pyrrolidine	Configuration at Carbon attached to R_1
1.		NH	H	S	RS
2		NH	H	S	RS
3.		O	H	S	RS
4.		O	H	S	RS
5.		O	H	S	RS
6.		O	H	S	RS
7.		O	H	S	RS
8.		O	H	S	RS
9.		O	CO	S	RS
10.		O	OH	S	RS
11.		O	H	S	RS
12.		O	H	S	RS
13.		O	H	S	RS
14.		O	H	S	RS
15.		O	H	S	R
16.		O	H	S	R
17.		O	H	S	R

10540245species





chain nodes :
7 13 14 15 16
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 17 18 19 20 21
ring/chain nodes :
23
chain bonds :
6-7 7-8 7-13 7-14 14-15 14-16 16-17 20-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19
19-20 20-21
exact/norm bonds :
7-13 8-9 8-12 9-10 10-11 11-12 14-15 14-16 16-17 17-18 17-21 18-19
19-20 20-21 20-23
exact bonds :
6-7 7-8 7-14
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 23:CLASS

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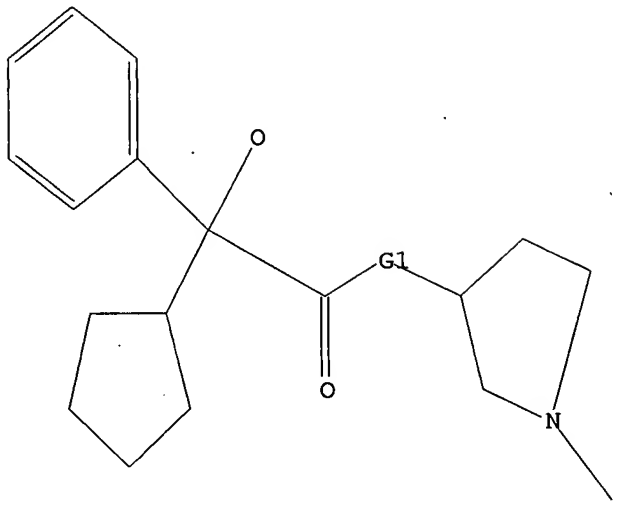
L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

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FULL SCREEN SEARCH COMPLETED - 540 TO ITERATE

100.0% PROCESSED 540 ITERATIONS 180 ANSWERS
SEARCH TIME: 00.00.01

L2 180 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'CAPLUS' ENTERED AT 11:56:03 ON 30 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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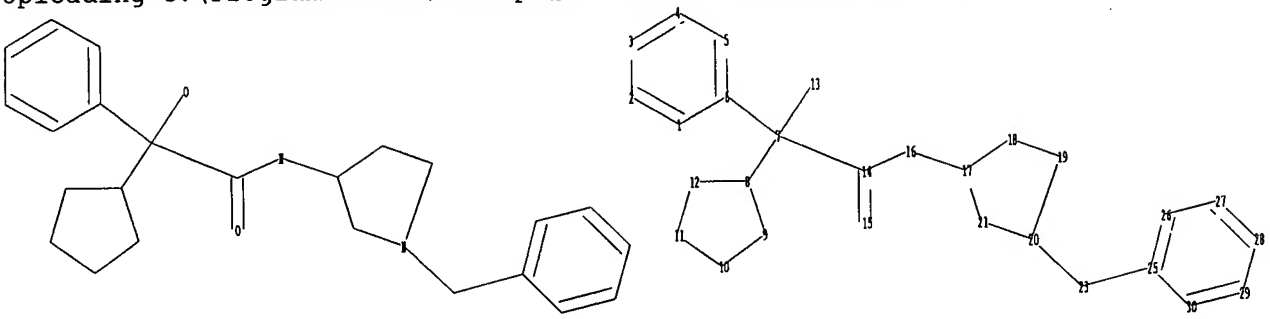

chain nodes :
7 13 14 15 16 23
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 17 18 19 20 21 25 26 27 28 29 30
chain bonds :
6-7 7-8 7-13 7-14 14-15 14-16 16-17 20-23 23-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19
19-20 20-21 25-26 25-30 26-27 27-28 28-29 29-30
exact/norm bonds :
7-13 14-15 14-16 16-17 19-20 20-21 20-23
exact bonds :
6-7 7-8 7-14 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19 23-25
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30
isolated ring systems :
containing 1 : 8 : 17 :

G1:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 23:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom

L4 STRUCTURE UPLOADED

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L4 HAS NO ANSWERS
L4 STR

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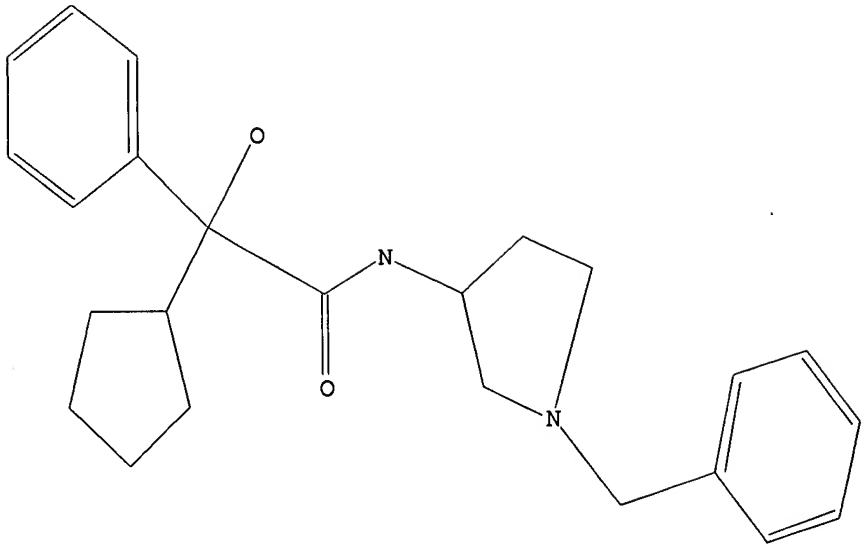

G1 O,N

Structure attributes must be viewed using STN Express query preparation.

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FULL SUBSET SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L5 1 SEA SUB=L2 SSS FUL L4

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	41.10	214.00

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FILE COVERS 1907 - 30 Apr 2007 VOL 146 ISS 19
FILE LAST UPDATED: 29 Apr 2007 (20070429/ED)

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=> s l5
L6   1 L5

=> d ibib abs hitstr tot

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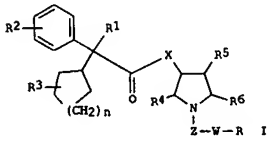
L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:546475 CAPLUS
DOCUMENT NUMBER: 141:106362
TITLE: Preparation of 1-substituted-3-pyrrolidine derivatives as muscarinic receptor antagonists
INVENTOR(S): Mehta, Anita; Gupta, Jang Bahadur; Sarma, Pakala Kumara Savithru
PATENT ASSIGNEE(S): Ranbaxy Laboratories Limited, India
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056767	A1	20040708	WO 2002-IB5590	20021223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002347552	A1	20040714	AU 2002-347552	20021223
EP 1583741	A1	20051012	EP 2002-783480	20021223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2006194862	A1	20060831	US 2006-540245	20060207
PRIORITY APPLN. INFO.:			WO 2002-IB5590 A	20021223

OTHER SOURCE(S): CASREACT 141:106362; MARPAT 141:106362
GI



I

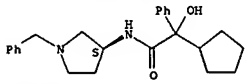
AB Title muscarinic receptor antagonists I (X = O, NH, etc.; R1 = OH, etc.; R2 = H, halo, alkyl; R3 = H, OH, etc.; R4, R5, R6 = H, alkyl; ; Z = CH2, SO2, carbonyl; W = alkylene, etc.; R = alkyl, aryl, etc.), useful for the treatment of various diseases of the respiratory, urinary and gastrointestinal systems mediated through muscarinic receptors, are prepared

L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
The affinity of these compds. for M2 and M3 muscarinic receptor subtype was tested. For example, (3S)-1-benzylpyrrolidin-3-yl cyclopentyl(hydroxy)phenylacetate was prepd. and had pKi = 6.13/7.17 for the M2 and M3 receptor subtype resp.

IT 719278-59-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 1-substituted-3-pyrrolidine derivs. as muscarinic receptor antagonists)

RN 719278-59-8 CAPLUS
CN Benzeneacetamide, α-cyclopentyl-α-hydroxy-N-[(3S)-1-(phenylmethyl)-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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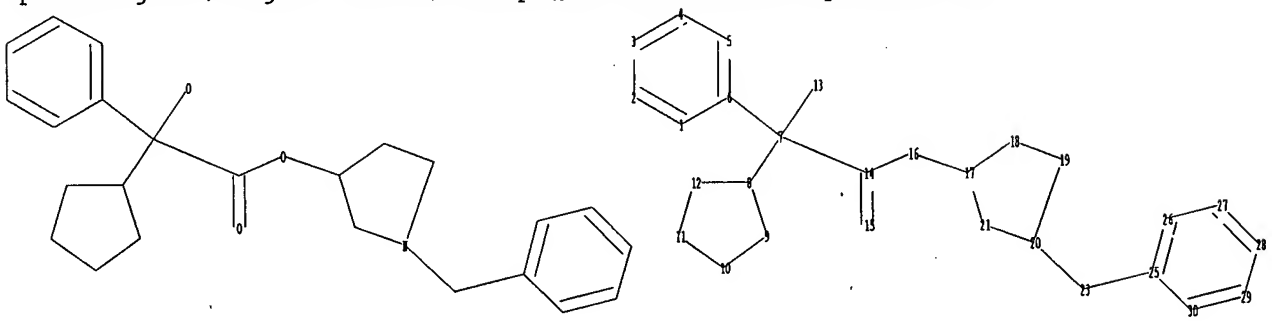

chain nodes :
7 13 14 15 16 23
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 17 18 19 20 21 25 26 27 28 29 30
chain bonds :
6-7 7-8 7-13 7-14 14-15. 14-16 16-17 20-23 23-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19
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containing 1 : 8 : 17 :

G1:O,N

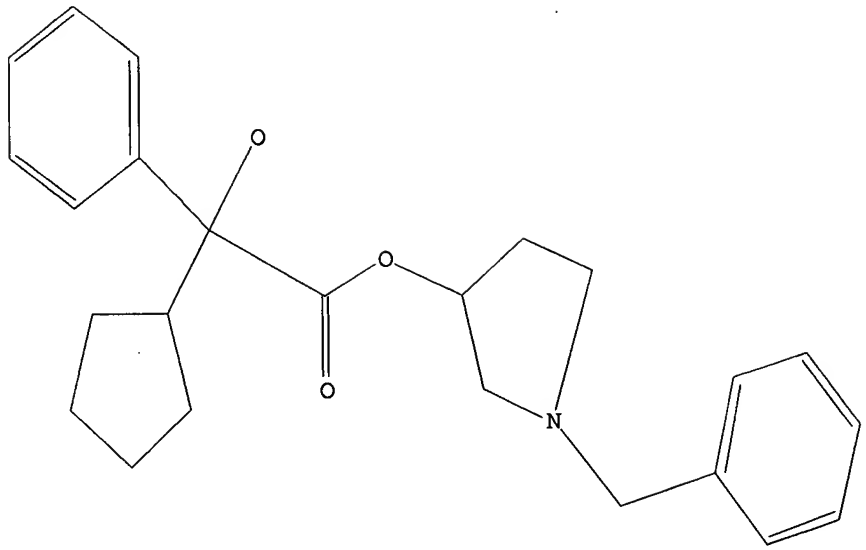
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 23:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom

L7 STRUCTURE UPLOADED

=> d
L7 HAS NO ANSWERS
L7 STR

Karen Cheng

10540245species



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=> s l7 full sub = l2
   REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 11:59:15 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 12 TO ITERATE

100.0% PROCESSED 12 ITERATIONS 8 ANSWERS
SEARCH TIME: 00.00.01

L8 8 SEA SUB=L2 SSS FUL L7

SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH
L9 3 L8

=> d ibib abs hitstr tot

Karen Cheng

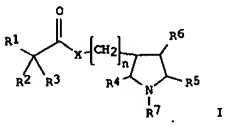
10540245species

L9 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:164888 CAPLUS
DOCUMENT NUMBER: 144:253999
TITLE: Preparation of pyrrolidine derivatives as muscarinic receptor antagonists
INVENTOR(S): Salman, Mohammad; Sarma, Pakala Kumara Savithru; Shelke, Sandeep Y.; Chugh, Anita; Gupta, Suman
PATENT ASSIGNEE(S): Ranbaxy Laboratories Limited, India
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006018708	A2	20060223	WO 2005-IB2449	20050818
WO 2006018708	A3	20060420		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: IN 2004-DE1550 A 20040819
IN 2005-DE1796 A 20050711
OTHER SOURCE(S): MARPAT 144:253999
GI

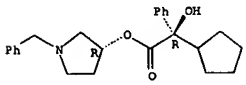


I

AB Title compds. I [R1, R2 = alkyl, alkenyl, alkynyl, etc.; R3 = H, alkyl, hydroxy, etc.; X = O, S, NR8; R8 = H, alkyl, aralkyl; n = 0-3; R4, R5, R6 = H, alkyl; R7 = H, alkyl, -(CH2)m-R11, etc.; R11 = aryl, heteroaryl; m = 1-3; with the proviso that R1, R2 and R3 can not be Ph, cycloalkyl and hydroxy, resp., when R9 and R10 are H and Ph, and with the further proviso that when R7 is (CH2)m-R11, R3 is H] and their pharmaceutically acceptable

L9 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
salts were prepd. For example, EDCI mediated amidation of 2-cyclopentyl-2-hydroxy-2-phenylacetic acid with (1-benzylpyrrolidin-3-ylmethyl)-methyl-amine afforded N-(1-benzylpyrrolidin-3-ylmethyl)-2-cyclopentyl-2-hydroxy-N-methyl-2-phenylacetamide in 75.3% yield. In M3 muscarinic receptor binding assays, 31 examples of compds. I exhibited the Ki value ranging from 1000 nM to 0.1 nM. Compds. I are claimed useful for the treatment of obesity, diabetes, etc.
IT 877172-67-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrrolidine derivs. as muscarinic receptor antagonists for
treatment of obesity, diabetes, etc.)
RN 877172-67-3 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3R)-1-(phenylmethyl)-3-pyrrolidinyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:546475 CAPLUS
DOCUMENT NUMBER: 141:106362
TITLE: Preparation of 1-substituted-3-pyrrolidine derivatives as muscarinic receptor antagonists
INVENTOR(S): Mehta, Anita; Gupta, Jang Bahadur; Sarma, Pakala Kumara Savithru
PATENT ASSIGNEE(S): Ranbaxy Laboratories Limited, India
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056767	A1	20040708	WO 2002-IB5590	20021223

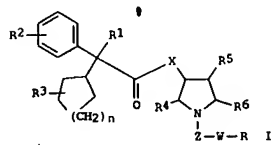
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2002347552	A1	20040714	AU 2002-347552	20021223
EP 1583741	A1	20051012	EP 2002-783480	20021223

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

US 2006194862	A1	20060831	US 2006-540245	20060207

PRIORITY APPLN. INFO.: WO 2002-IB5590 A 20021223
OTHER SOURCE(S): CASREACT 141:106362; MARPAT 141:106362
GI

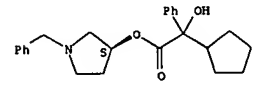


I

AB Title muscarinic receptor antagonists I (X = O, NH, etc.; R1 = OH, etc.; R2 = H, halo, alkyl; R3 = H, OH, etc.; R4, R5, R6 = H, alkyl; ; Z = CH2, SO2, carbonyl; W = alkylene, etc.; R = alkyl, aryl, etc.), useful for the treatment of various diseases of the respiratory, urinary and gastrointestinal systems mediated through muscarinic receptors, are prepared The affinity of these compds. for M2 and M3 muscarinic receptor subtype was tested. For example, (3S)-1-benzylpyrrolidin-3-yl cyclopentyl(hydroxy)phenylacetate was prepared and had pKi = 6.13/7.17 for the M2 and M3 receptor subtype resp.

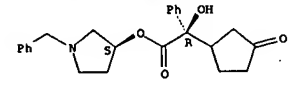
L9 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 719278-61-2P 719278-67-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 1-substituted-3-pyrrolidine derivs. as muscarinic receptor
antagonists)
RN 719278-61-2 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-(phenylmethyl)-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



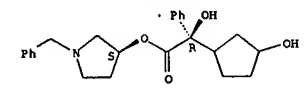
RN 719278-67-8 CAPLUS
CN Benzeneacetic acid, α-hydroxy-α-(3-oxocyclopentyl)-, (3S)-1-(phenylmethyl)-3-pyrrolidinyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 719278-68-9P 719278-73-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-substituted-3-pyrrolidine derivs. as muscarinic receptor
antagonists)
RN 719278-68-9 CAPLUS
CN Benzeneacetic acid, α-hydroxy-α-(3-hydroxycyclopentyl)-, (3S)-1-(phenylmethyl)-3-pyrrolidinyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 719278-73-6 CAPLUS

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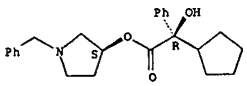
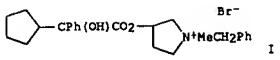
L9 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-(phenylmethyl)-3-pyrrolidinyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:130844 CAPLUS
DOCUMENT NUMBER: 88:130844
TITLE: The control of cardiac arrhythmias with O-substituted pyrrolidinols
AUTHOR(S): Koppanyi, Theodore
CORPORATE SOURCE: Georgetown Univ., Washington, DC, USA
SOURCE: Congr. Hung. Pharmacol. Soc., [Proc.] (1976), Volume Date 1974, 2(6, Symp. Pharmacol. Heart), 53-7
CODEN: CPSPDT
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

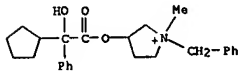


I

AB Both 1-benzyl-3-pyrrolidyl acetate methobromide [52-61-9] and 1-benzyl-3-pyrrolidyl α-phenylcyclopentaneglycolate methobromide (I) [65976-16-1] exibited antiarrhythmic effects in isolated heart prepns. (from rabbits and rats) and in dogs. These compds. are not cardiac depressant drugs, and they had low acute and subacute toxicities. These compds. appear to be effective in the management of both atrial and ventricular ectopic rhythms. The compds. antagonized both the muscarinic and nicotinic stimulation of the heart, suggesting that the 2 receptor sites are the same or similar.

IT 65976-16-1
RL: BIOL (Biological study)
(antiarrhythmic)

RN 65976-16-1 CAPLUS
CN Pyrrolidinium, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-1-methyl-1-(phenylmethyl)-, bromide (9CI) (CA INDEX NAME)



● Br⁻

10540245species

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	17.69	279.00

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.34	-3.12

FILE 'REGISTRY' ENTERED AT 12:01:51 ON 30 APR 2007
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 29 APR 2007 HIGHEST RN 933681-85-7
DICTIONARY FILE UPDATES: 29 APR 2007 HIGHEST RN 933681-85-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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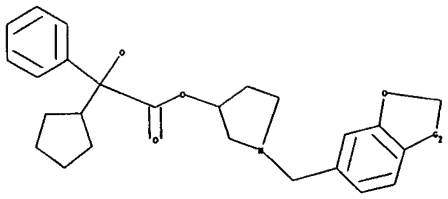
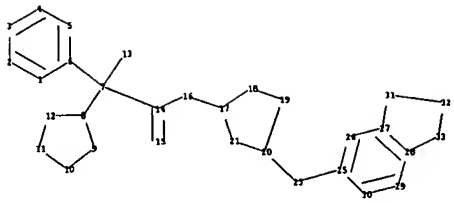
Karen Cheng

10540245species





chain nodes :
7 13 14 15 16 23
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 17 18 19 20 21 25 26 27 28 29 30 31 32 33
chain bonds :
6-7 7-8 7-13 7-14 14-15 14-16 16-17 20-23 23-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19 19-20 20-21 25-26 25-30 26-27 27-28 27-31 28-29 28-33 29-30 31-32 32-33
exact/norm bonds :
6-7 7-8 7-13 7-14 8-9 8-12 9-10 10-11 11-12 14-15 14-16 16-17 17-18 17-21 18-19 19-20 20-21 20-23 23-25 27-31 28-33 31-32 32-33
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30
isolated ring systems :
containing 1 : 8 : 17 :

G1:O,N

G2:C,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 23:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom

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10540245species

L10 STRUCTURE UPLOADED

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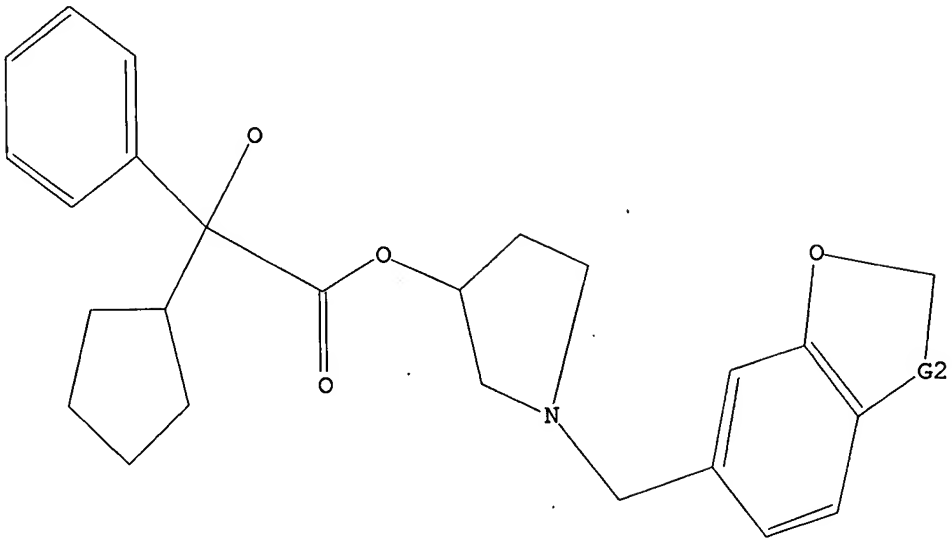
ENTER LOGIC EXPRESSION, QUERY NAME, OR (END):end
SEARCH ENDED BY USER

=> d
L10 HAS NO ANSWERS
L10 STR



G1 O,N
G2 C,O

Structure attributes must be viewed using STN Express query preparation.

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FULL SUBSET SEARCH INITIATED 12:02:15 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L11 0 SEA SUB=L2 SSS FUL L10

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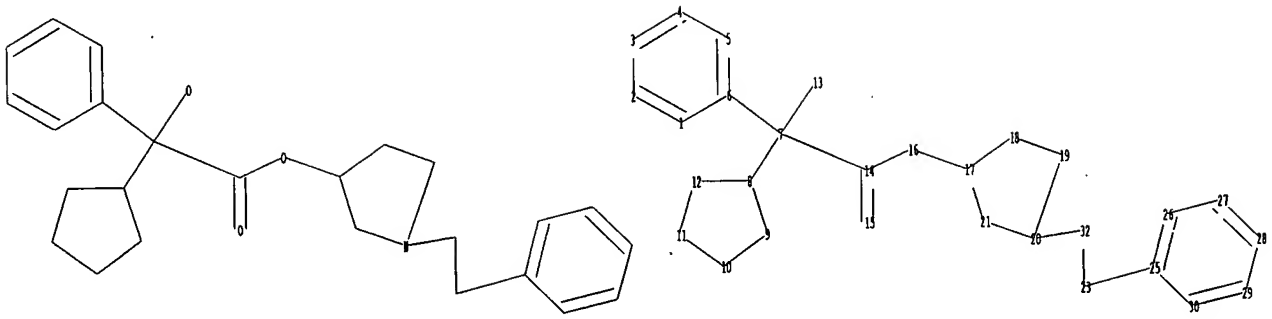
10540245species



chain nodes :
7 13 14 15 16 23 32
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 17 18 19 20 21 25 26 27 28 29 30
chain bonds :
6-7 7-8 7-13 7-14 14-15 14-16 16-17 20-32 23-25 23-32
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19
19-20 20-21 25-26 25-30 26-27 27-28 28-29 29-30
exact/norm bonds :
7-13 14-15 14-16 16-17 19-20 20-21 20-32
exact bonds :
6-7 7-8 7-14 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19 23-25 23-32
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30
isolated ring systems :
containing 1 : 8 : 17 :

G1:O,N

G2:C,O

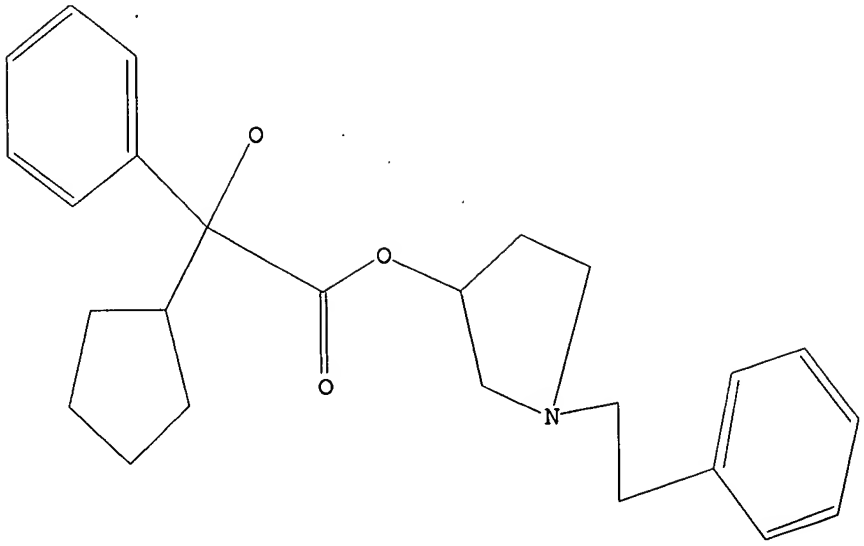
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 23:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
32:CLASS

L12 STRUCTURE UPLOADED

=> d
L12 HAS NO ANSWERS
L12 STR

Karen Cheng

10540245species



G1 O,N
G2 C,O

Structure attributes must be viewed using STN Express query preparation.

=> s l12 full
FULL SEARCH INITIATED 12:04:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 96 TO ITERATE

100.0% PROCESSED 96 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

L13 5 SEA SSS FUL L12

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	214.10	493.10

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.12

FILE 'CAPLUS' ENTERED AT 12:04:04 ON 30 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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10540245species

FILE COVERS 1907 - 30 Apr 2007 VOL 146 ISS 19
FILE LAST UPDATED: 29 Apr 2007 (20070429/ED)

=> s l13
L14 1 L13

=> d ibib abs hitstr tot

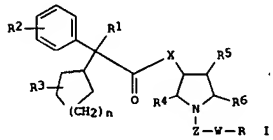
Karen Cheng

10540245species

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:546475 CAPLUS
DOCUMENT NUMBER: 141:106362
TITLE: Preparation of 1-substituted-3-pyrrolidine derivatives as muscarinic receptor antagonists
INVENTOR(S): Mehta, Anita; Gupta, Jang Bahadur; Sarma, Pakala Kumara Savithru
PATENT ASSIGNEE(S): Ranbaxy Laboratories Limited, India
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056767	A1	20040708	WO 2002-IB5590	20021223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002347552	A1	20040714	AU 2002-347552	20021223
EP 1583741	A1	20051012	EP 2002-783480	20021223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2006194862	A1	20060831	US 2006-540245	20060207

PRIORITY APPLN. INFO.: WO 2002-IB5590 A 20021223
OTHER SOURCE(S): CASREACT 141:106362; MARPAT 141:106362
GI



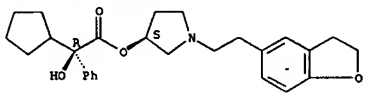
I

AB Title muscarinic receptor antagonists I (X = O, NH, etc.; R1 = OH, etc.; R2 = H, halo, alkyl; R3 = H, OH, etc.; R4, R5, R6 = H, alkyl; ; Z = CH2, SO2, carbonyl; W = alkylene, etc.; R = alkyl, aryl, etc.), useful for the treatment of various diseases of the respiratory, urinary and gastrointestinal systems mediated through muscarinic receptors, are prepared

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

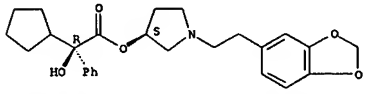
RN 719278-74-7 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[2-(2,3-dihydro-5-benzofuranyl)ethyl]-3-pyrrolidinyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 719278-75-8 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[2-(1,3-benzodioxol-5-yl)ethyl]-3-pyrrolidinyl ester, (αR)- (9CI) (CA INDEX NAME)

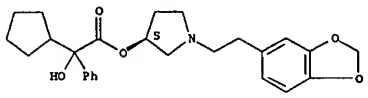
Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

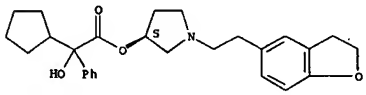
L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
The affinity of these compds. for M2 and M3 muscarinic receptor subtype was tested. For example, (3S)-1-benzylpyrrolidin-3-yl cyclopentyl(hydroxy)phenylacetate was prepd. and had pKi = 6.13/7.17 for the M2 and M3 receptor subtype resp.
IT 719278-62-3P 719278-63-4P 719278-69-0P
719278-74-7P 719278-75-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-substituted-3-pyrrolidine derivs. as muscarinic receptor antagonists)
RN 719278-62-3 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[2-(1,3-benzodioxol-5-yl)ethyl]-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



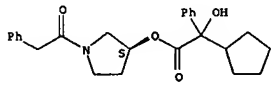
RN 719278-63-4 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[2-(2,3-dihydro-5-benzofuranyl)ethyl]-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 719278-69-0 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-(phenylacetyl)-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



Karen Cheng

10540245species

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	9.50	502.60

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.78	-3.90

FILE 'REGISTRY' ENTERED AT 12:09:35 ON 30 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 APR 2007 HIGHEST RN 933681-85-7
DICTIONARY FILE UPDATES: 29 APR 2007 HIGHEST RN 933681-85-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

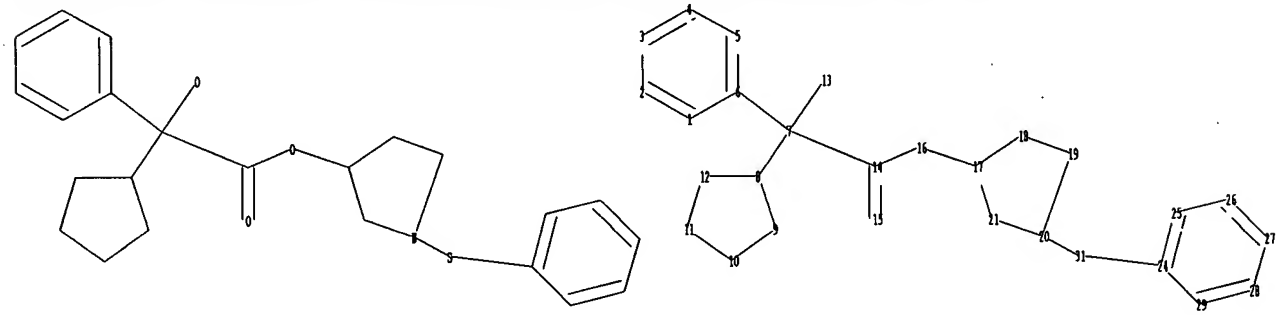
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10540245species5.str



chain nodes :
7 13 14 15 16 31

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10540245species

ring nodes :
1 2 3 4 5 6 8 9 10 11 12 17 18 19 20 21 24 25 26 27 28 29
chain bonds :
6-7 7-8 7-13 7-14 14-15 14-16 16-17 20-31 24-31
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19
19-20 20-21 24-29 24-25 25-26 26-27 27-28 28-29
exact/norm bonds :
7-13 14-15 14-16 16-17 19-20 20-21 20-31 24-31
exact bonds :
6-7 7-8 7-14 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 24-29 24-25 25-26 26-27 27-28 28-29
isolated ring systems :
containing 1 : 8 : 17 :

G1:O,N

G2:C,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:CLASS

L15 STRUCTURE UPLOADED

=> d
L15 HAS NO ANSWERS
L15 STR

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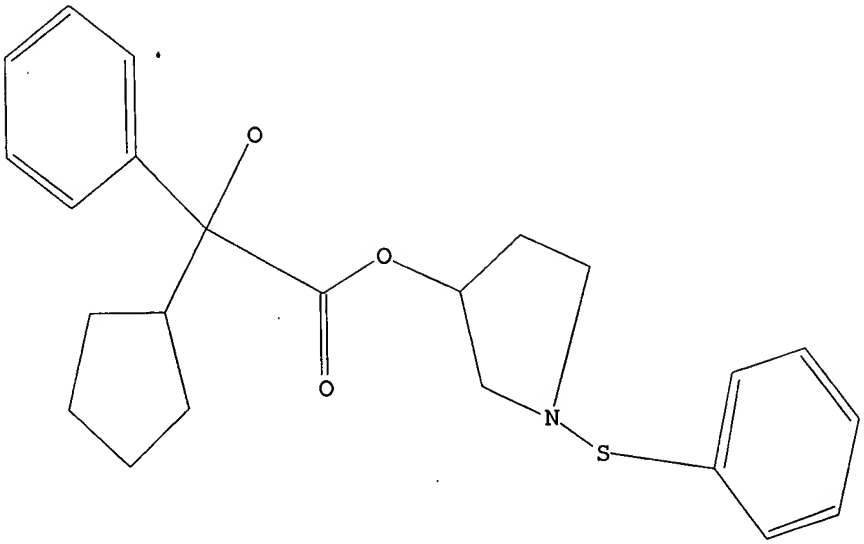
10540245species



G1 O,N
G2 C,O

Structure attributes must be viewed using STN Express query preparation.

=> s l15 full
FULL SEARCH INITIATED 12:09:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 552 TO ITERATE

100.0% PROCESSED 552 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

L16 3 SEA SSS FUL L15

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	674.70

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.90

FILE 'CAPLUS' ENTERED AT 12:09:56 ON 30 APR 2007
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10540245species

FILE COVERS 1907 - 30 Apr 2007 VOL 146 ISS 19
FILE LAST UPDATED: 29 Apr 2007 (20070429/ED)

=> s l16
L17 1 L16

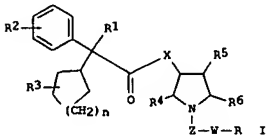
=> d ibib abs hitstr tot

Karen Cheng

L17 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:546475 CAPLUS
DOCUMENT NUMBER: 141:106362
TITLE: Preparation of 1-substituted-3-pyrrolidine derivatives as muscarinic receptor antagonists
INVENTOR(S): Mehta, Anita; Gupta, Jang Bahadur; Sarma, Pakala Kumara Savithru
PATENT ASSIGNEE(S): Ranbaxy Laboratories Limited, India
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

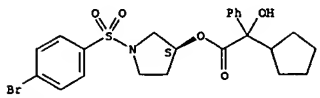
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056767	A1	20040708	WO 2002-IB5590	20021223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002347552	A1	20040714	AU 2002-347552	20021223
EP 1583741	A1	20051012	EP 2002-783480	20021223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2006194862	A1	20060831	US 2006-540245	20060207
PRIORITY APPLN. INFO.:			WO 2002-IB5590 A	20021223

OTHER SOURCE(S): CASREACT 141:106362; MARPAT 141:106362
GI



AB Title muscarinic receptor antagonists I (X = O, NH, etc.; R1 = OH, etc.; R2 = H, halo, alkyl; R3 = H, OH, etc.; R4, R5, R6 = H, alkyl; ; Z = CH2, SO2, carbonyl; W = alkylene, etc.; R = alkyl, aryl, etc.), useful for the treatment of various diseases of the respiratory, urinary and gastrointestinal systems mediated through muscarinic receptors, are prepared

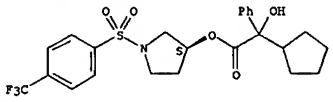
L17 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

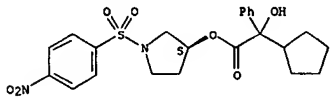
L17 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
The affinity of these compds. for M2 and M3 muscarinic receptor subtype was tested. For example, (3S)-1-benzylpyrrolidin-3-yl cyclopentyl(hydroxy)phenylacetate was prepd. and had pKi = 6.13/7.17 for the M2 and M3 receptor subtype resp.
IT 719278-65-6P 719278-66-7P 719278-72-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-substituted-3-pyrrolidine derivs. as muscarinic receptor antagonists)
RN 719278-65-6 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[[4-(trifluoromethyl)phenyl]sulfonyl]-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 719278-66-7 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[(4-nitrophenyl)sulfonyl]-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 719278-72-5 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[(4-bromophenyl)sulfonyl]-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10540245species

=> fil reg
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 8.56 | 683.26

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION
CA SUBSCRIBER PRICE | -0.78 | -4.68

FILE 'REGISTRY' ENTERED AT 12:14:25 ON 30 APR 2007
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 APR 2007 HIGHEST RN 933681-85-7
DICTIONARY FILE UPDATES: 29 APR 2007 HIGHEST RN 933681-85-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10540245species6.str

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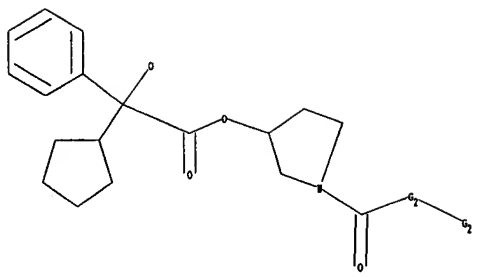
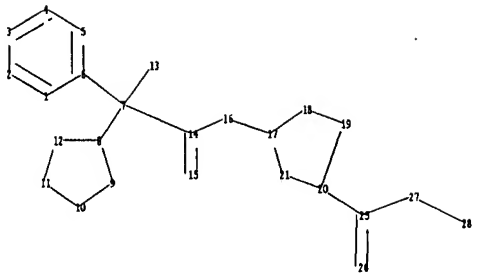
10540245species





chain nodes :
7 13 14 15 16 25 26 27 28
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 17 18 19 20 21
chain bonds :
6-7 7-8 7-13 7-14 14-15 14-16 16-17 20-25 25-26 25-27 27-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19
19-20 20-21
exact/norm bonds :
7-13 14-15 14-16 16-17 19-20 20-21 20-25 25-26 25-27 27-28
exact bonds :
6-7 7-8 7-14 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 8 : 17 :

G1:O,N

G2:C,O

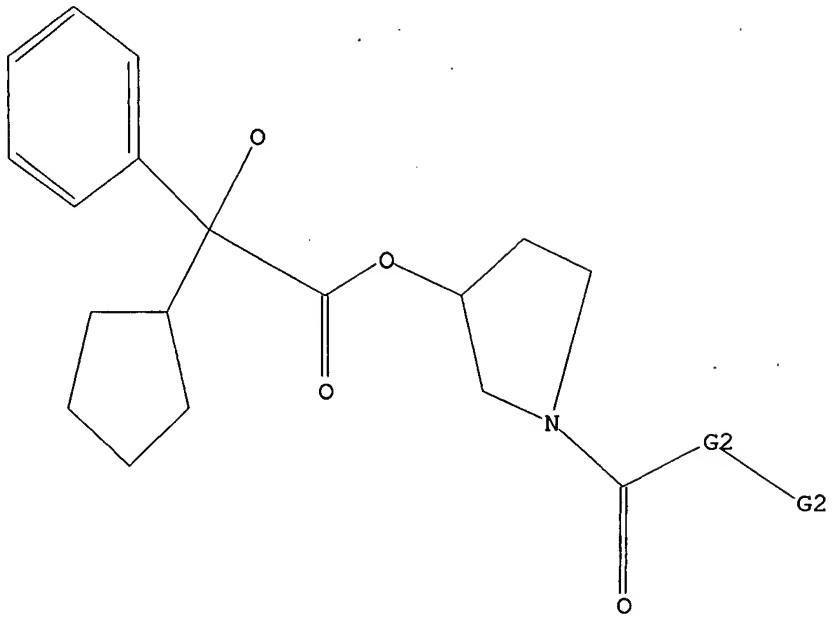
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS

Karen Cheng

10540245species

L18 STRUCTURE UPLOADED

=> d
L18 HAS NO ANSWERS
L18 STR



G1 O,N
G2 C,O

Structure attributes must be viewed using STN Express query preparation.

=> s l8 full
FULL SEARCH INITIATED 12:15:09 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 50 TO ITERATE

100.0% PROCESSED 50 ITERATIONS 8 ANSWERS
SEARCH TIME: 00.00.01

L19 8 SEA SSS FUL L7

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.10 855.36

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION

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10540245species

```
=> s l18 full
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



FULL SEARCH INITIATED 12:17:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       42 TO ITERATE

100.0% PROCESSED       42 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

L21            3 SEA SSS FUL L18


L22           2 L21

=> d ibib abs hitstr tot
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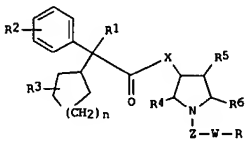
Karen Cheng

L22 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:546475 CAPLUS
DOCUMENT NUMBER: 141:106362
TITLE: Preparation of 1-substituted-3-pyrrolidine derivatives as muscarinic receptor antagonists
INVENTOR(S): Mehta, Anita; Gupta, Jang Bahadur; Sarma, Pakala Kumara Savithru
PATENT ASSIGNEE(S): Ranbaxy Laboratories Limited, India
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056767	A1	20040708	WO 2002-IB5590	20021223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002347552	A1	20040714	AU 2002-347552	20021223
EP 1583741	A1	20051012	EP 2002-783480	20021223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2006194862	A1	20060831	US 2006-540245	20060207
PRIORITY APPLN. INFO.:			WO 2002-IB5590 A	20021223
OTHER SOURCE(S):			CASREACT 141:106362; MARPAT 141:106362	

GI



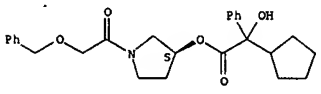
AB Title muscarinic receptor antagonists I (X = O, NH, etc.; R1 = OH, etc.; R2 = H, halo, alkyl; R3 = H, OH, etc.; R4, R5, R6 = H, alkyl; , Z = CH2, SO2, carbonyl; W = alkylene, etc.; R = alkyl, aryl, etc.), useful for the

L22 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
treatment of various diseases of the respiratory, urinary and gastrointestinal systems mediated through muscarinic receptors, are prepd. The affinity of these compds. for M2 and M3 muscarinic receptor subtype was tested. For example, (3S)-1-benzylpyrrolidin-3-yl cyclopentyl(hydroxy)phenylacetate was prepd. and had pKi = 6.13/7.17 for the M2 and M3 receptor subtype resp.

IT 719278-70-3P 719278-71-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-substituted-3-pyrrolidine derivs. as muscarinic receptor antagonists)

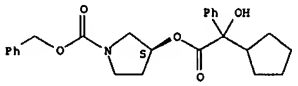
RN 719278-70-3 CAPLUS
CN Benzeneacetic acid, α-cyclopentyl-α-hydroxy-, (3S)-1-[(phenylmethoxy)acetyl]-3-pyrrolidinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 719278-71-4 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, 3-[(cyclopentylhydroxyphenylacetyl)oxy]-, phenylmethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:51415 CAPLUS
DOCUMENT NUMBER: 136:118468
TITLE: Preparation of 2-aryl-2-hydroxyacetic acid ester derivatives as muscarinic M3 receptor antagonists
INVENTOR(S): Ogino, Yoshio; Kurihara, Hideki; Matsuda, Kenji; Numazawa, Tomoshige; Otake, Norikazu; Noguchi, Kazuhito
PATENT ASSIGNEE(S): Banyu Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 138 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004402	A1	20020117	WO 2001-JP5987	20010710
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 200171027	A	20020121	AU 2001-71027	20010710
CA 2415468	A1	20030110	CA 2001-2415468	20010710
EP 1302458	A1	20030416	EP 2001-949925	20010710
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003191316	A1	20031009	US 2003-332617	20030110
US 6846835	B2	20050125		
US 2005065211	A1	20050324	US 2004-983613	20041109
US 7192969	B2	20070320		
PRIORITY APPLN. INFO.:			JP 2000-210591 A	20000711
			WO 2001-JP5987 W	20010710
			US 2003-332617 A3	20030110
OTHER SOURCE(S):			MARPAT 136:118468	

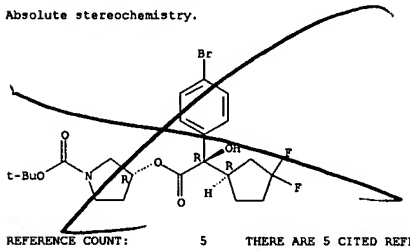
AB Compds. of the general formula ArC(OH)(R1)CO2A [wherein A is a group of the general formula -B1-N+R2R3R4.X- or -B2-NR5CR6:NR7; Ar is aryl or heteroaryl, any of which may be substituted; B1 and B2 are each an aliphatic hydrocarbon group; R1 is fluorinated cycloalkyl; R2, R3 and R4 are each lower alkyl, or a single bond or alkylene, any of which is bonded to B1, or alternatively R2 and R3 may be united to form alkylene; R5 and R7 are each hydrogen, lower alkyl, or a single bond or alkylene, any of which is bonded to B2; R6 is hydrogen, lower alkyl, or N(R8)R9; R8 and R9 are independently hydrogen or lower alkyl; and X- is an anion] are prepared Thses compds. exhibit selective muscarinic M3 receptor antagonism with little side effects and are suitable for administration by inhalation and useful as therapeutic agents for respiratory system diseases including chronic obstructive pulmonary diseases, chronic bronchitis, asthma, chronic airway obstruction, pulmonary fibrosis, pulmonary emphysema, or rhinitis. Thus, reductive methylation of piperidin-4-yl (2R)-((1R)-3,3-difluoropentyl)-2-hydroxy-2-phenylethanoate by formaldehyde and sodium cyanoborohydride in the presence of ZnCl2 in MeOH at room temperature
for 30 min gave 1-methylpiperidin-4-yl (2R)-((1R)-3,3-difluoropentyl)-2-

L22 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
hydroxy-2-phenylethanoate which was quaternized by Me bromide in MeCN at room temp. for 15 h to give 4-[[(2R)-2-((1R)-3,3-difluorocyclopentyl)-2-hydroxy-2-phenylethanoyl]oxy]-1,1-dimethylpiperidinium bromide (I). In a muscarinic receptor M2 and M3 antagonism assay, 4-(((2R)-2-((1R)-3,3-difluorocyclopentyl)-2-hydroxy-2-phenylethanoyl)oxy)-1,1-dimethylpiperidinium bromide in vitro exhibited KB of 9.6 nM for inhibiting the carbachol-induced redn. in heart beat in rat right atrium (muscarinic receptor M2 receptor) and that of 0.004 nM for inhibiting the carbachol-induced contraction of trachea (muscarinic receptor M3 receptor) with M2/M3 receptor ratio of 218. An ampule or a powder inhalation formulation contg. I were described.

IT 389890-48-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylhydroxyacetic acid ester derivs. as muscarinic M3 receptor antagonists for therapeutic agents)

RN 389890-48-6 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, 3-[[(2R)-(4-bromophenyl)[(1R)-3,3-difluorocyclopentyl]hydroxyacetyl]oxy]-, 1,1-dimethylethyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10540245species

=> fil reg
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 11.48 | 1056.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION
CA SUBSCRIBER PRICE | -1.56 | -8.58

FILE 'REGISTRY' ENTERED AT 12:18:45 ON 30 APR 2007
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 APR 2007 HIGHEST RN 933681-85-7
DICTIONARY FILE UPDATES: 29 APR 2007 HIGHEST RN 933681-85-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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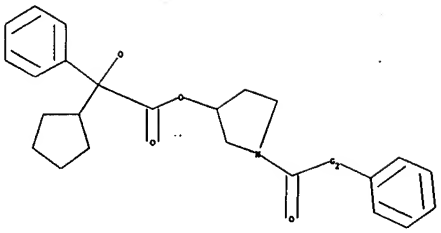
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

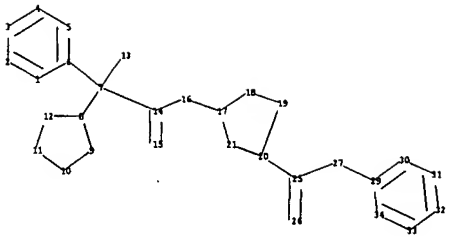
http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10540245species7.str

Karen Cheng

10540245species





chain nodes :
7 13 14 15 16 25 26 27
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 17 18 19 20 21 29 30 31 32 33 34
chain bonds :
6-7 7-8 7-13 7-14 14-15 14-16 16-17 20-25 25-26 25-27 27-29
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19
19-20 20-21 29-30 29-34 30-31 31-32 32-33 33-34
exact/norm bonds :
7-13 14-15 14-16 16-17 19-20 20-21 20-25 25-26 25-27 27-29
exact bonds :
6-7 7-8 7-14 8-9 8-12 9-10 10-11 11-12 17-18 17-21 18-19
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 29-30 29-34 30-31 31-32 32-33 33-34
isolated ring systems :
containing 1 : 8 : 17 :

G1:O,N

G2:C,O

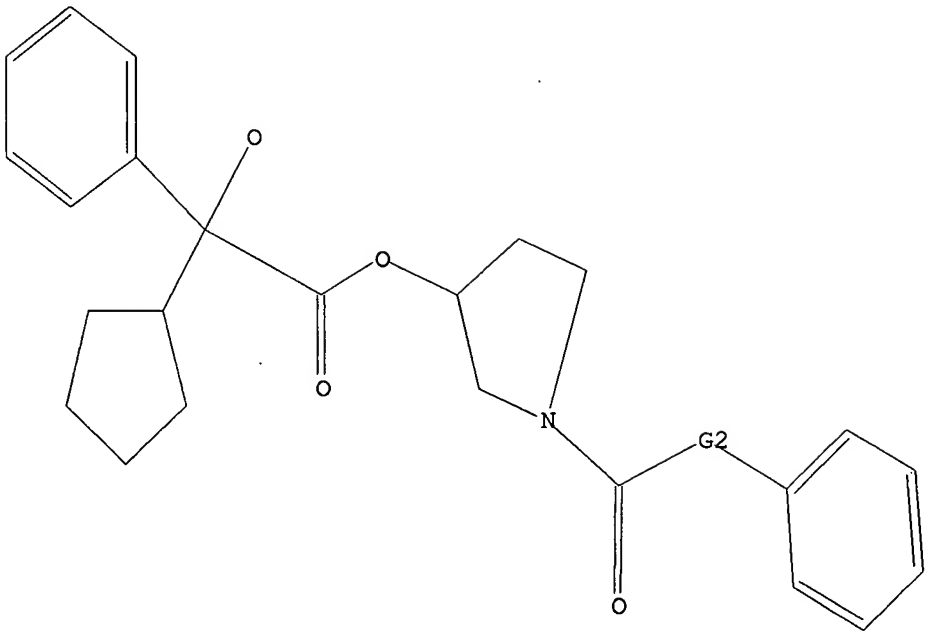
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 25:CLASS 26:CLASS 27:CLASS 29:CLASS 30:Atom 31:Atom
32:Atom 33:Atom 34:CLASS

Karen Cheng

10540245species

L23 STRUCTURE UPLOADED

=> d
L23 HAS NO ANSWERS
L23 STR



G1 O,N
G2 C,O

Structure attributes must be viewed using STN Express query preparation.

=> s l23 full
FULL SEARCH INITIATED 12:19:16 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L24 1 SEA SSS FUL L23

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.10 1228.26

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

Karen Cheng